Application No.: 10/691,095
Amendment Date: February 2, 2010
Reply to Office Action of September 2, 2009

**AMENDMENTS TO THE CLAIMS:**

This listing of claims will replace all prior versions, and listings, of claims in the application:

**Claim 1 (Currently Amended):** A method of treating migraine, epilepsy, or bipolar disorder in a mammal comprising administering to a mammal a therapeutically effective amount of a compound of formula (I)

(I),

or a pharmaceutically acceptable prodrug thereof, wherein

A is cyclohexyl optionally substituted with 1, 2, 3, or 4 alkyl groups ~~cycloalkyl or bicycloalkyl~~;

$R_A$, $R_B$, and $R_C$ are independently hydrogen or alkyl;

$R_1$ is $OR_3$ or $NR_3R_4$;

$R_2$ is hydrogen, ~~alkyl, aryl, arylalkyl, cycloalkyl, cycloalkylalkyl, heterocycle, or heterocycloalkyl~~;

$R_3$ and $R_4$ are independently hydrogen, ~~alkenyl, alkyl, alkynyl, alkoxycarbonylalkyl, aryl, arylalkyl,~~ carboxyalkyl, ~~cycloalkyl, cycloalkylalkyl, heterocycle, heterocycloalkyl,~~ hydroxyalkyl, ~~$(NR_5R_6)$alkyl,~~ or $(NR_5R_6)$carbonylalkyl, ~~or~~

~~]]; or~~

~~$R_3$ and $R_4$ taken together with the nitrogen atom to which they are attached form a heterocycle wherein the heterocycle is azepanyl, azetidinyl, aziridinyl, morpholinyl, piperazinyl, piperidinyl, pyrrolidinyl, or thiomorpholinyl~~; and

# Author Search

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=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 14:43:11 ON 28 APR 2010
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 28 Apr 2010  VOL 152 ISS 18
FILE LAST UPDATED: 27 Apr 2010  (20100427/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED:  Feb 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE:  Feb 2010

HCAplus now includes complete International Patent Classification (IPC)
reclassification data for the first quarter of 2010.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.
'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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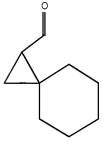


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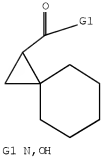


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=> D IBIB ED ABS HITSTR L21 1-2

L21  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2004:857165  HCAPLUS  Full-text
DOCUMENT NUMBER:          141:325759
TITLE:                    Spirocyclopropyl amides and acids and their
                          therapeutic applications
INVENTOR(S):              Bennani, Youseff L.; Bunnelle, William          abandoned
                          H.; Chang, Sou-Jen; Chemburkar,
                          Sanjay R.; Chen, Jinhua; Dart,
                          Michael J.; Fernando, Dilinie; Ku,
                          Yi-Yin; Lockwood, Mark; Wang,
                          Lei
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 27 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.          DATE
     --------------      ----   --------    -------------------      --------
     US 20040204396       A1    20041014    US 2003-691095           20031022 <--
PRIORITY APPLN. INFO.:                      US 2002-420286P      P   20021022 <--
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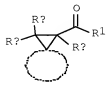
OTHER SOURCE(S): MARPAT 141:325759
ED Entered STN: 18 Oct 2004
GI



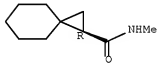

I

AB The present invention relates to the use of compds. I (A = cycloalkyl or bicycloalkyl; RA, RB, RC = H, alkyl; R1 = OR2, NR3R4; R2 = H, alkyl, aryl, arylalkyl, cycloalkyl, cycloalkylalkyl, heterocycle, heterocyclealkyl; R3, R4 = H, alkenyl, alkyl, etc.) for the treatment of epilepsy, bipolar disorder, psychiatric disorders, migraine, pain, or movement disorders, and to provide neuroprotection. Representative compds. exhibited anticonvulsant ED50s in the range of about 0.36 mmol/kg to about 0.20 mmol/kg using the maximal electroshock procedure with mice. Many compds. were prepared and are claimed.

IT 1055761-02-8 1055761-03-9
RL: PRPH (Prophetic)
(Spirocyclopropyl amides and acids and their therapeutic applications)

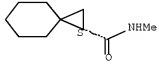
RN 1055761-02-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-methyl-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



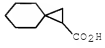

RN 1055761-03-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-methyl-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



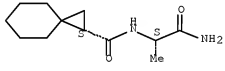

IT 17202-86-7P, Spiro[2.5]octane-1-carboxylic acid
680618-92-2P, (1S)-N-((1S)-2-Amino-1-methyl-2-oxoethyl)spiro[2.5]octane-1-carboxamide 680618-93-3P, (1R)-N-((1S)-2-Amino-1-methyl-2-oxoethyl)spiro[2.5]octane-1-carboxamide

680618-94-4P 680618-96-6P 680619-02-7P,
2-Methylspiro[2.5]octane-1-carboxylic acid 680619-04-9P,
5,7-Dimethylspiro[2.5]octane-1-carboxylic acid 680619-06-1P,
6-tert-Butylspiro[2.5]octane-1-carboxylic acid 680619-24-3P
680619-41-4P, 5,5,7,7-Tetramethylspiro[2.5]octane-1-carboxylic
acid
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); RACT (Reactant or reagent); USES
(Uses)
(spirocyclopropyl amides and acids for neuroprotection and treatment of
epilepsy, bipolar disorders, migraine,)
RN 17202-86-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid (CA INDEX NAME)



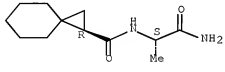
RN 680618-92-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(1S)-2-amino-1-methyl-2-oxoethyl]-,
(1S)- (CA INDEX NAME)

Absolute stereochemistry.



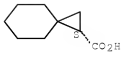
RN 680618-93-3 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(1S)-2-amino-1-methyl-2-oxoethyl]-,
(1R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680618-94-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680618-96-6 HCAPLUS
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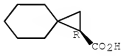
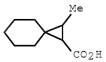
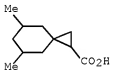
Absolute stereochemistry.



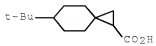
RN 680619-02-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-methyl- (CA INDEX NAME)



RN 680619-04-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 5,7-dimethyl- (CA INDEX NAME)

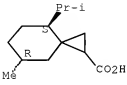


RN 680619-06-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 6-(1,1-dimethylethyl)- (CA INDEX NAME)

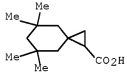


RN 680619-24-3 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 7-methyl-4-(1-methylethyl)-, (4S,7R)-
(CA INDEX NAME)

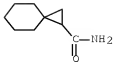
Absolute stereochemistry.




RN 680619-41-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 5,5,7,7-tetramethyl- (CA INDEX NAME)




IT 17202-88-9P, Spiro[2.5]octane-1-carboxamide
680618-91-1P, N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide
680618-95-5P, (1S)-N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide 680619-03-8P,
N-(2-Amino-2-oxoethyl)-2-methylspiro[2.5]octane-1-carboxamide
680619-05-0P, N-(2-Amino-2-oxoethyl)-5,7-dimethylspiro[2.5]octane-1-carboxamide 680619-07-2P,
N-(2-Amino-2-oxoethyl)-6-tert-butylspiro[2.5]octane-1-carboxamide
680619-26-5P 680619-28-7P 680619-37-8P,
N-(3-Amino-3-oxopropyl)spiro[2.5]octane-1-carboxamide
680619-43-6P, 5,5,7,7-Tetramethylspiro[2.5]octane-1-carboxamide
680619-45-8P, N-(2-Amino-2-oxoethyl)-5,5,7,7-tetramethylspiro[2.5]octane-1-carboxamide 680619-47-0P,
[(Spiro[2.5]oct-1-ylcarbonyl)amino]acetic acid 680619-54-9P,
(1R)-N-((2R)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide
680619-55-0P, (1S)-N-((2R)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide 680619-56-1P,
(1R)-N-((2S)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide
680619-57-2P, (1S)-N-((2S)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(spirocyclopropyl amides and acids for neuroprotection and treatment of epilepsy, bipolar disorders, migraine,)
RN 17202-88-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide (CA INDEX NAME)



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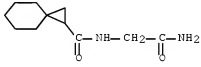
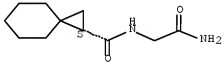
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)- (CA INDEX NAME)

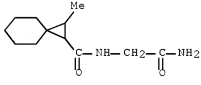


RN 680618-95-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-, (1S)- (CA INDEX NAME)

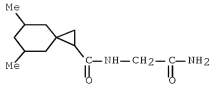
Absolute stereochemistry.



RN 680619-03-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-2-methyl- (CA INDEX NAME)



RN 680619-05-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-5,7-dimethyl- (CA INDEX NAME)



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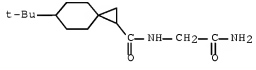
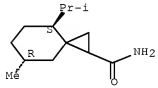
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-6-(1,1-dimethylethyl)- (CA INDEX NAME)



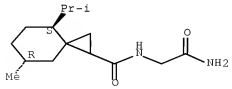
RN 680619-26-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 7-methyl-4-(1-methylethyl)-, (4S,7R)- (CA INDEX NAME)

Absolute stereochemistry.

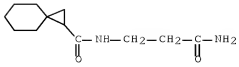


RN 680619-28-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-7-methyl-4-(1-methylethyl)-, (4S,7R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-37-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(3-amino-3-oxopropyl)- (CA INDEX NAME)



RN 680619-43-6 HCAPLUS
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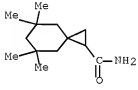

RN 680619-45-8 HCAPLUS
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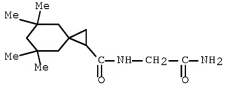
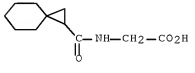
(CA INDEX NAME)

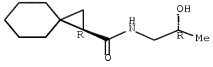


RN 680619-47-0 HCAPLUS
CN Glycine, N-(spiro[2.5]oct-1-ylcarbonyl)- (CA INDEX NAME)



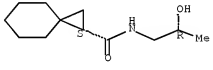
RN 680619-54-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(2R)-2-hydroxypropyl]-, (1R)- (CA
INDEX NAME)

Absolute stereochemistry.



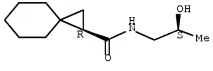
RN 680619-55-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(2R)-2-hydroxypropyl]-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



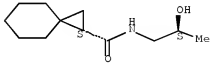
RN 680619-56-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(2S)-2-hydroxypropyl]-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-57-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(2S)-2-hydroxypropyl]-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

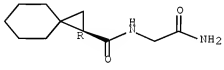


IT 680618-97-7, (1R)-N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide 680619-58-3 680619-59-4
680619-60-7, 2-Methylspiro[2.5]octane-1-carboxamide

680619-61-8, 5,7-Dimethylspiro[2.5]octane-1-carboxamide
680619-62-9, 6-tert-Butylspiro[2.5]octane-1-carboxamide
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(spirocyclopropyl amides and acids for neuroprotection and treatment of epilepsy, bipolar disorders, migraine,)

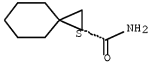
RN 680618-97-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



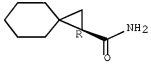
RN 680619-58-3 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

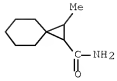


RN 680619-59-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-60-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 2-methyl- (CA INDEX NAME)



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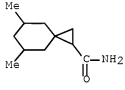
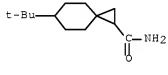


RN 680619-62-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



L21 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2004:331780 HCAPLUS Full-text
DOCUMENT NUMBER: 140:338974
TITLE: Preparation of spirocyclopropyl amides and acids as anticonvulsants
INVENTOR(S): Bennani, Youssef L.; Bunnelle, William H.; Chang, Scu-Jen; Chemburkar, Sanjay R.; Chen, Jinhua; Dart, Michael J.; Fernando, Dilinie P.; Ku, Yi-Yin; Lockwood, Mark; Wang, Lei
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 27 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 20040077616 | A1 | 20040422 | US 2002-277266 | 20021022 <-- |

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     WO 2004037240        A1    20040506    WO 2003-US33688         20031022 <--
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             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
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PRIORITY APPLN. INFO.:                       US 2002-277266      A   20021022 <--
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ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S):         MARPAT 140:338974
ED   Entered STN:  23 Apr 2004
GI
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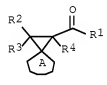


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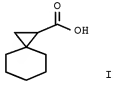


II

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AB   Title compds. I [A = cycloalkyl, bicycloalkyl; R2-4 = H, alkyl; R1 = alkoxy,
     amino] are prepared  For instance, methylenecyclohexane is treated with Et
     diazoacetate (methylcyclohexane, Cu, 100-105°) and the resulting ester
     saponified to give II.  Representative examples of I exhibit ED50 = 0.84 -
     0.35 mmol/kg in the s.c. pentylenetetrazole (PTZ) seizure model.  I are useful
     in the treatment of epilepsy, bipolar disorder, psychiatric disorders,
     migraine, pain, or movement disorders, and to provide neuroprotection.
IT   1055761-02-8   1055761-03-9
     RL: PRPH (Prophetic)
         (Preparation of spirocyclopropyl amides and acids as anticonvulsants)
RN   1055761-02-8  HCAPLUS
CN   Spiro[2.5]octane-1-carboxamide, N-methyl-, (1R)-  (CA INDEX NAME)

Absolute stereochemistry.
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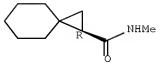
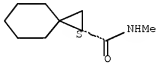


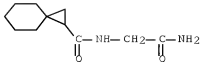

RN 1055761-03-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-methyl-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



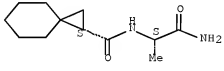

IT 17202-86-7P, Spiro[2.5]octane-1-carboxylic acid
680618-91-1P, N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide
680618-92-2P, (1S)-N-((1S)-2-Amino-1-methyl-2-oxoethyl)spiro[2.5]octane-1-carboxamide 680618-93-3P, (1R)-N-((1S)-2-Amino-1-methyl-2-oxoethyl)spiro[2.5]octane-1-carboxamide
680618-94-4P, (S)-Spiro[2.5]octane-1-carboxylic acid
680618-96-6P, (R)-Spiro[2.5]octane-1-carboxylic acid
680619-02-7P, 2-Methylspiro[2.5]octane-1-carboxylic acid
680619-04-9P, 5,7-Dimethylspiro[2.5]octane-1-carboxylic acid
680619-06-1P, 6-tert-Butylspiro[2.5]octane-1-carboxylic acid
680619-24-3P 680619-41-4P,
5,5,7,7-Tetramethylspiro[2.5]octane-1-carboxylic acid
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of spirocyclopropyl amides and acids as anticonvulsants)
RN 17202-86-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid (CA INDEX NAME)


RN 680618-91-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)- (CA INDEX NAME)



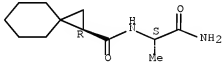
RN 680618-92-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(1S)-2-amino-1-methyl-2-oxoethyl]-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



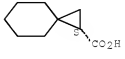
RN 680618-93-3 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(1S)-2-amino-1-methyl-2-oxoethyl]-, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



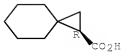
RN 680618-94-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

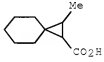


RN 680618-96-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, (1R)- (CA INDEX NAME)

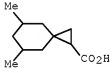
Absolute stereochemistry.



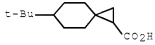
RN 680619-02-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-methyl- (CA INDEX NAME)



RN 680619-04-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 5,7-dimethyl- (CA INDEX NAME)

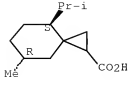


RN 680619-06-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



RN 680619-24-3 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 7-methyl-4-(1-methylethyl)-, (4S,7R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-41-4 HCAPLUS
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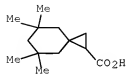

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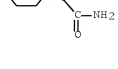
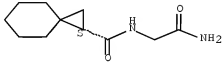
680618-95-5P, (1S)-N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide 680618-97-7P,
(1R)-N-(2-Amino-2-oxoethyl)spiro[2.5]octane-1-carboxamide
680619-03-8P, N-(2-Amino-2-oxoethyl)-2-methylspiro[2.5]octane-1-carboxamide 680619-05-0P,
N-(2-Amino-2-oxoethyl)-5,7-dimethylspiro[2.5]octane-1-carboxamide
680619-07-2P, N-(2-Amino-2-oxoethyl)-6-tert-butylspiro[2.5]octane-1-carboxamide 680619-26-5P 680619-28-7P
680619-37-8P, N-(3-Amino-3-oxopropyl)spiro[2.5]octane-1-carboxamide 680619-43-6P,
5,5,7,7-Tetramethylspiro[2.5]octane-1-carboxamide 680619-45-8P
, N-(2-Amino-2-oxoethyl)-5,5,7,7-tetramethylspiro[2.5]octane-1-carboxamide
680619-47-0P, [(Spiro[2.5]oct-1-ylcarbonyl)amino]acetic acid
680619-49-2P, (S)-[[Spiro[2.5]oct-1-ylcarbonyl]amino]acetic acid
680619-51-6P, (R)-[[Spiro[2.5]oct-1-ylcarbonyl]amino]acetic acid
680619-54-9P, (1R)-N-((2R)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide 680619-55-0P,
(1S)-N-((2R)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide
680619-56-1P, (1R)-N-((2S)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide 680619-57-2P,
(1S)-N-((2S)-2-Hydroxypropyl)spiro[2.5]octane-1-carboxamide
680619-58-3P, (S)-Spiro[2.5]octane-1-carboxamide
680619-59-4P, (R)-Spiro[2.5]octane-1-carboxamide
680619-60-7P, 2-Methylspiro[2.5]octane-1-carboxamide
680619-61-8P, 5,7-Dimethylspiro[2.5]octane-1-carboxamide
680619-62-9P, 6-tert-Butylspiro[2.5]octane-1-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of spirocyclopropyl amides and acids as anticonvulsants)
RN 17202-88-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide (CA INDEX NAME)



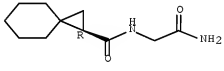
RN 680618-95-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.

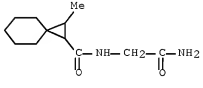


RN 680618-97-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-, (1R)- (CA INDEX NAME)

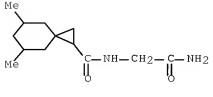
Absolute stereochemistry.



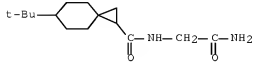
RN 680619-03-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-2-methyl- (CA INDEX NAME)



RN 680619-05-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-5,7-dimethyl- (CA INDEX NAME)

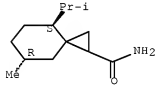


RN 680619-07-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-6-(1,1-dimethylethyl)- (CA INDEX NAME)



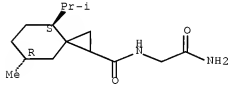
RN 680619-26-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 7-methyl-4-(1-methylethyl)-, (4S,7R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-28-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-7-methyl-4-(1-methylethyl)-, (4S,7R)- (CA INDEX NAME)

Absolute stereochemistry.



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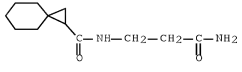

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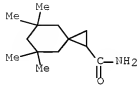
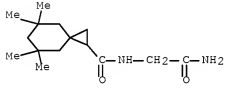


RN 680619-45-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(2-amino-2-oxoethyl)-5,5,7,7-tetramethyl-
(CA INDEX NAME)



RN 680619-47-0 HCAPLUS
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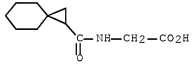
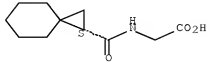


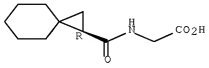
RN 680619-49-2 HCAPLUS
CN Glycine, N-[(1S)-spiro[2.5]oct-1-ylcarbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-51-6 HCAPLUS
CN Glycine, N-[(1R)-spiro[2.5]oct-1-ylcarbonyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 680619-54-9 HCAPLUS
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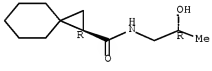
Absolute stereochemistry.



RN 680619-55-0 HCAPLUS
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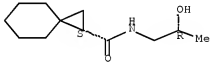
Absolute stereochemistry.



RN 680619-56-1 HCAPLUS
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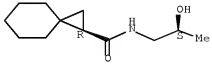
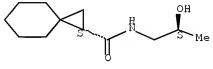
Absolute stereochemistry.



RN 680619-57-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-[(2S)-2-hydroxypropyl]-, (1S)- (CA INDEX NAME)

Absolute stereochemistry.



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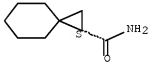
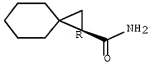
Absolute stereochemistry.



RN 680619-59-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, (1R)- (CA INDEX NAME)

Absolute stereochemistry.



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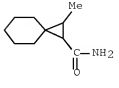
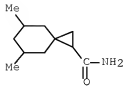
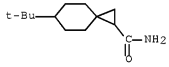


RN 680619-61-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 5,7-dimethyl- (CA INDEX NAME)




RN 680619-62-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 6-(1,1-dimethylethyl)- (CA INDEX NAME)



# Structure Search

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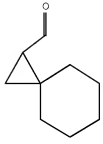

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Structure attributes must be viewed using STN Express query preparation.
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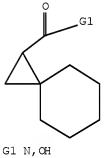


G1 N,OH

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Structure attributes must be viewed using STN Express query preparation.
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                 DISORDERS"+OLD,NT/CT OR MIGRAINE+OLD,NT/CT OR EPILEPSY+OLD,NT/
                CT
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=> S L23 NOT L21
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=> D IBIB ED ABS HITSTR L24 1

L24  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2004:467697  HCAPLUS  Full-text                Bad date*
DOCUMENT NUMBER:          141:38623
TITLE:                    A preparation of fused bicyclic nitrogen-containing
                          heterocycles, useful in the treatment or prevention of
```

metabolic and cell proliferative diseases
INVENTOR(S): Fox, Brian M.; Furukawa, Noboru; Hao, Xiaolin; Iio, Kiyosei; Inaba, Takashi; Jackson, Simon M.; Kayser, Frank; Labelle, Marc; Li, Kexue; Matsui, Takuya; McMinn, Dustin L.; Ogawa, Nobuya; Rubenstein, Steven M.; Sagawa, Shoichi; Sugimoto, Kazuyuki; Suzuki, Masahiro; Tanaka, Masahiro; Ye, Guosen; Yoshida, Atsuhito; Zhang, Jian
PATENT ASSIGNEE(S): Tularik Inc., USA; Japan Tobacco, Inc.
SOURCE: PCT Int. Appl., 176 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004047755 | A2 | 20040610 | WO 2003-US37574 | 20031121 <-- |
| WO 2004047755 | A3 | 20041125 | | |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
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| CA 2514473 | C | 20080527 | | |
| AU 2003293006 | A1 | 20040618 | AU 2003-293006 | 20031121 <-- |
| US 20040209871 | A1 | 20041021 | US 2003-720844 | 20031121 <-- |
| US 7244727 | B2 | 20070717 | | |
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| BR 2003015688 | A | 20050906 | BR 2003-15688 | 20031121 <-- |
| JP 2006509764 | T | 20060323 | JP 2004-555693 | 20031121 <-- |
| JP 3988830 | B2 | 20071010 | | |
| CN 1753897 | A | 20060329 | CN 2003-80109107 | 20031121 <-- |
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| RU 2342388 | C2 | 20081227 | RU 2005-119646 | 20031121 <-- |
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| KR 772297 | B1 | 20071102 | KR 2005-709128 | 20050520 <-- |
| IN 2005DN02477 | A | 20070126 | IN 2005-DN2477 | 20050609 <-- |
| NO 2005002923 | A | 20050818 | NO 2005-2923 | 20050615 <-- |
| US 20070244096 | A1 | 20071018 | US 2007-743376 | 20070502 <-- |
| PRIORITY APPLN. INFO.: | | | US 2002-428600P P | 20021122 <-- |
| | | | US 2003-720844 A3 | 20031121 |
| | | | WO 2003-US37574 W | 20031121 |

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 141:38623
ED Entered STN: 10 Jun 2004
GI

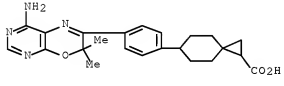
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to fused bicyclic nitrogen-containing heterocycles of formula I [wherein: X is C(R6) or N; Y is C(R6)1-2, N(R6)0-1; Z is O or S; W1 and W2 are independently selected from (un)substituted (hetero)cycloalkyl or (hetero)aryl; L1 and L2 are independently selected from bond, alkylene, or alkenylene, etc.; R1, R2, R3, and R4 are independently selected from H, alk(en/yn)yl, CHO, or C(O)-alkyl, etc.; R3 and R4 may be combined with the nitrogen to form a 5-, 6-, or 7-membered rings; R5 is H, (halo)alkyl, alk(en/yn)yl, OH, or alkoxy, etc.; R6 is H, alk(en/yn)yl, fluoroalkyl, or aryl, etc.], useful in the treatment or prevention of metabolic and cell proliferative diseases. The invention provides compds. which modulate the activity of proteins involved in lipid metabolism and cell proliferation. For instance, pyrimidine derivative II (hDGAT1 IC50 < 0.01 μM) was prepared via heterocyclization of 4,5-diamino-6-hydroxypyrimidine and bromoketone III (example 2, no yield data).

IT 701236-48-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of fused bicyclic nitrogen-containing heterocycles, useful in the
treatment or prevention of metabolic and cell proliferative diseases)

RN 701236-48-8 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 6-[4-(4-amino-7,7-dimethyl-7H-pyrimido[4,5-b][1,4]oxazin-6-yl)phenyl]- (CA INDEX NAME)




OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (21 CITINGS)

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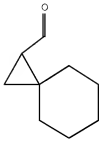

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Structure attributes must be viewed using STN Express query preparation.
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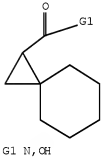


G1 N,OH

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Structure attributes must be viewed using STN Express query preparation.
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L10          41 SEA FILE=HCAPLUS SPE=ON  ABB=ON  PLU=ON  L9 AND (PRY<=2002 OR
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=> S L10 NOT L21,L23
L25         38 L10 NOT (L21 OR L23)

=> D IBIB ED ABS HITSTR 1-38

L25  ANSWER 1 OF 38  HCAPLUS  COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER:         2008:1383602  HCAPLUS  Full-text
DOCUMENT NUMBER:          149:555106
TITLE:                    Intermolecular metal-catalyzed carbenoid
                          cyclopropanations
AUTHOR(S):                Davies, Huw M. L.; Antoulinakis, Evan G.
CORPORATE SOURCE:         State University of New York at Buffalo, Buffalo, NY,
                          USA
SOURCE:                   Organic Reactions (Hoboken, NJ, United States) (
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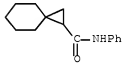
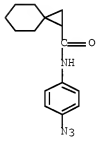
2001), 57, No pp. given
CODEN: ORHNBA
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 149:555106
ED Entered STN: 19 Nov 2008
AB A review of the article Intermol. metal-catalyzed carbenoid cyclopropanations.
IT 17202-89-0P 105311-14-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Intermol. Metal-Catalyzed Carbenoid Cyclopropanations)
RN 17202-89-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-phenyl- (CA INDEX NAME)

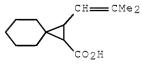



RN 105311-14-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(4-azidophenyl)- (CA INDEX NAME)

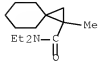



L25 ANSWER 2 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2008:1383595 HCAPLUS Full-text bad date (2005,not 1982
DOCUMENT NUMBER: 149:555101 as this appears to be)
TITLE: Allylic and benzylic carbanions substituted by heteroatoms
AUTHOR(S): Biellmann, Jean-Francois; Ducep, Jean-Bernard
CORPORATE SOURCE: Strasbourg, Fr.
SOURCE: Organic Reactions (Hoboken, NJ, United States) (1982), 27, No pp. given
CODEN: ORHNBA
URL: http://www3.interscience.wiley.com/cgi-bin/mrwhome/107610747/HOME
PUBLISHER: John Wiley & Sons, Inc.
DOCUMENT TYPE: Journal; General Review; (online computer file)
LANGUAGE: English

OTHER SOURCE(S): CASREACT 149:555101
ED Entered STN: 19 Nov 2008
AB A review of the article Allylic and benzylic carbanions substituted by heteroatoms.
IT 26069-11-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Allylic and Benzylic Carbanions Substituted by Heteroatoms)
RN 26069-11-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-(2-methyl-1-propen-1-yl)- (CA INDEX NAME)

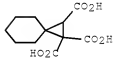



L25 ANSWER 3 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:471580 HCAPLUS Full-text
DOCUMENT NUMBER: 137:310623
TITLE: Complete stereospecific cyclopropanation of α,β-unsaturated amides promoted by Sm/CH2I2
AUTHOR(S): Concellon, Jose M.; Rodriguez-Solla, Humberto; Gomez, Cecilia
CORPORATE SOURCE: Departmento de Quimica Organica e Inorganica Facultad de Quimica, Universidad de Oviedo, Oviedo, 33071, Spain
SOURCE: Angewandte Chemie, International Edition (2002), 41(11), 1917-1919
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:310623
ED Entered STN: 24 Jun 2002
AB Complete stereospecific cyclopropanation of α,β-unsatd. amides R1CR2:CR3CONR42, in which the double bond is di-, tri-, or tetrasubstituted, is promoted by Sm/CH2I2. The reaction is high yielding and unaffected by the bulk of the substituents R1-R4.
IT 471278-64-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereospecific cyclopropanation of α,β-unsatd. amides promoted by Sm/CH2I2)
RN 471278-64-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N,N-diethyl-1-methyl- (CA INDEX NAME)



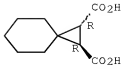
OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)
REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 4 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1995:401083 HCAPLUS Full-text
DOCUMENT NUMBER: 123:169252
ORIGINAL REFERENCE NO.: 123:30203a,30206a
TITLE: Synthesis of pyrethrin precursors and methylene lactones by decarboxylation of 1,1,2-cyclopropanetricarboxylic acids
AUTHOR(S): Benayache, S.; Benayache, F.; Jullien, R. F.; Wanat, M.
CORPORATE SOURCE: Inst. Chimie, Univ. de Constantine, Constantine, 25000, Algeria
SOURCE: Journal de la Societe Algerienne de Chimie ( 1992), 2(2), 99-110
CODEN: JSACEX; ISSN: 1111-4797
PUBLISHER: Societe Algerienne de Chimie
DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 08 Mar 1995
AB Cyclopropanetricarboxylic acids underwent decarboxylation in aprotic solvents. Cyclopropane ring opening occurs under acidic conditions. Thus, 3,3-dimethyl-1,1,2-cyclopropanetricarboxylic acid was treated with NaH in HMPT or 10% $H_2SO_4$ to afford cis- and trans-3,3-dimethyl-1,2-cyclopropanedicarboxylic acid or γ,γ-dimethyl-α,β-dicarboxy-γ-butyrolactone, resp.
IT 1021-30-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of pyrethrin precursors and methylene lactones by decarboxylation of cyclopropanetricarboxylic acids)
RN 1021-30-3 HCAPLUS
CN Spiro[2.5]octane-1,1,2-tricarboxylic acid (CA INDEX NAME)



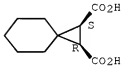

IT 67911-20-0P 68194-50-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of pyrethrin precursors and methylene lactones by decarboxylation of cyclopropanetricarboxylic acids)
RN 67911-20-0 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

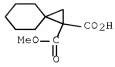


RN 68194-50-3 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, cis- (9CI) (CA INDEX NAME)

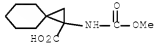
Relative stereochemistry.



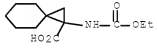
L25 ANSWER 5 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1995:231440 HCAPLUS Full-text
DOCUMENT NUMBER: 122:10523
ORIGINAL REFERENCE NO.: 122:2337a,2340a
TITLE: Straightforward Synthesis of 1-Amino-2,2-dialkylcyclopropanecarboxylic Acids via Selective Saponification of 2,2-Dialkylcyclopropane-1,1-dicarboxylic Esters and Curtius Rearrangement
AUTHOR(S): De Kimpe, Norbert; Boeykens, Marc; Tehrani, Kourosch Abbaspour
CORPORATE SOURCE: Faculty of Agricultural and Applied Biological Sciences, University of Gent, Ghent, B-9000, Belg.
SOURCE: Journal of Organic Chemistry (1994), 59(26), 8215-19
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:10523
ED Entered STN: 08 Dec 1994
AB Selective monosaponification of di-Me 2,2-dialkylcyclopropane-1,1-dicarboxylic esters afforded the corresponding 2,2-dialkyl-1-(methoxycarbonyl)cyclopropane-1-carboxylic acids, which were rearranged with di-Ph phosphoroazidate via a modified Curtius-type reaction to give Me 2,2-dialkyl-1-(N-(alkoxycarbonyl)amino)cyclopropanecarboxylic esters. Selective deprotection of the carbamate or Me cyclopropanecarboxylic ester was worked out, giving rise to a whole variety of aminocyclopropanecarboxylate analogs.
IT 159279-66-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(straightforward synthesis of amino(dialkyl)cyclopropanecarboxylic acids via selective saponification of diesters and Curtius rearrangement)
RN 159279-66-0 HCAPLUS
CN Spiro[2.5]octane-1,1-dicarboxylic acid, 1-methyl ester (CA INDEX NAME)



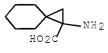
IT 159279-75-1P 159279-76-2P 159279-82-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(straightforward synthesis of amino(dialkyl)cyclopropanecarboxylic acids via selective saponification of diesters and Curtius rearrangement)
RN 159279-75-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-[(methoxycarbonyl)amino]- (CA INDEX NAME)



RN 159279-76-2 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-[(ethoxycarbonyl)amino]- (CA INDEX NAME)



RN 159279-82-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-amino- (CA INDEX NAME)



OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (18 CITINGS)

L25 ANSWER 6 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1993:448977 HCAPLUS Full-text
DOCUMENT NUMBER: 119:48977
ORIGINAL REFERENCE NO.: 119:8869a,8872a
TITLE: Surface nature of Grignard reagent formation. Chiral 1-methylspiro[2.5]octylmagnesium bromide

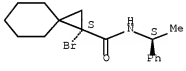
AUTHOR(S): Hamdouchi, C.; Topolski, M.; Goedken, V.; Walborsky, H. M.
CORPORATE SOURCE: Dittmer Lab. Chem., Florida State Univ., Tallahassee, FL, 32306, USA
SOURCE: Journal of Organic Chemistry (1993), 58(11), 3148-55
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:48977
ED Entered STN: 07 Aug 1993
GI


I

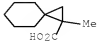
AB The synthesis of chiral 1-bromo-1-methylspiro[2.5]octane (I) is described. The absolute configuration of I has been established as (S)-(+). From stereochem., product anal., and radical trapping expts. it is concluded that the reaction of chiral I with magnesium to form the corresponding Grignard reagent occurs mainly on the surface of the magnesium.

IT 148065-45-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal and mol. structure of)
RN 148065-45-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-bromo-N-(1-phenylethyl)-, [S-(R*,R*)]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

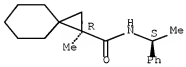



IT 42077-50-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with chiral α-methylbenzylamine)
RN 42077-50-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-methyl- (CA INDEX NAME)



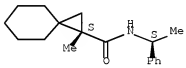
IT 148065-43-0P 148601-33-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 148065-49-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-N-(1-phenylethyl)-, [S-(R*,S*)]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 148601-33-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-N-(1-phenylethyl)-, [S-(R*,R*)]-
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

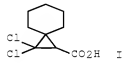



IT 148065-44-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, resolution, reduction and amidation of)
RN 148065-44-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-bromo- (CA INDEX NAME)


OS.CITING REF COUNT: 17 THERE ARE 17 CAPLUS RECORDS THAT CITE THIS RECORD (17 CITINGS)

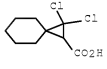
L25 ANSWER 7 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1991:43192 HCAPLUS Full-text
DOCUMENT NUMBER: 114:43192
ORIGINAL REFERENCE NO.: 114:7525a,7528a
TITLE: Synthesis of potent pyrethroids: α(RS)-cyano-4-fluoro-benzyl/3-phenoxybenzyl 2,2-dichloro-spiro (2,5)-octane-1-carboxylates
AUTHOR(S): Sattar, A. K.; Arbale, A. A.; Kulkarni, G. H.

CORPORATE SOURCE: Natl. Chem. Lab., Pune, 411 008, India
SOURCE: Synthetic Communications (1990), 20(14), 2217-23
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:43192
ED Entered STN: 09 Feb 1991
GI

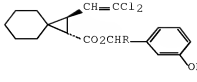



I

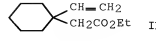
AB A simple facile synthesis of 2,2-dichloro-spiro (2,5)-octane-1-carboxylic acid (I) was described. I was converted into the corresponding α-(RS) cyano 3-phenoxybenzyl ester, exhibiting high insecticidal activity against Musca domestica and Aedes egyptii.
IT 131447-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and correlation or esterification of)
RN 131447-79-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2,2-dichloro- (CA INDEX NAME)



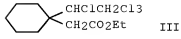

L25 ANSWER 8 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1989:192300 HCAPLUS Full-text
DOCUMENT NUMBER: 110:192300
ORIGINAL REFERENCE NO.: 110:31909a,31912a
TITLE: Synthesis of insecticidally active 3-phenoxybenzyl and α-(RS)-cyano-3-phenoxybenzyl (±)-trans-2-(2,2-dichlorovinyl)spiro[2.5]octane-1-carboxylates
AUTHOR(S): Kulkarni, G. H.; Arbale, A. A.
CORPORATE SOURCE: Natl. Chem. Lab., Pune, India
SOURCE: Synthetic Communications (1988), 18(16-17), 2147-59
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:192300
ED Entered STN: 26 May 1989
GI



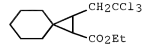
I



II



III



IV

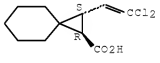
AB The preparation of the title compds. I (R = H, cyano) from cyclohexanone and Ph3P:CHCO2Et is reported. Key reactions include the condensation-Claisen rearrangement of cyclohexylideneethanol with MeC(OEt)3 to give (vinylcyclohexyl)acetate II and the ring closure of [(tetrachloropropyl)cyclohexyl]acetate III to give trichloroethylspirooctanecarboxylate IV.

IT 120368-79-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to acid chloride)

RN 120368-79-8 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 2-(2,2-dichloroethenyl)-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.

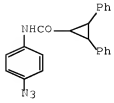


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

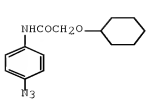
L25 ANSWER 9 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN

| | |
|---|---|
| ACCESSION NUMBER: | 1987:84111 HCAPLUS Full-text |
| DOCUMENT NUMBER: | 106:84111 |
| ORIGINAL REFERENCE NO.: | 106:13793a,13796a |
| TITLE: | Selective reactions of azide-substituted α-diazo amides with olefins and alcohols using rhodium(II) catalysts |
| AUTHOR(S): | Jeganathan, Alwarsamy; Richardson, Stewart K.; Mani, Rajarathnam S.; Haley, Boyd E.; Watt, David S. |
| CORPORATE SOURCE: | Lucille Parker Markey Cancer Cent., Univ. Kentucky, Lexington, KY, 40506, USA |
| SOURCE: | Journal of Organic Chemistry (1986), 51(26), 5362-7<br>CODEN: JOCEAH; ISSN: 0022-3263 |
| DOCUMENT TYPE: | Journal |
| LANGUAGE: | English |
| OTHER SOURCE(S): | CASREACT 106:84111 |

ED Entered STN: 21 Mar 1987
GI




II

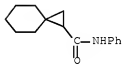



III

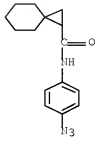
AB The synthesis and addition of azide-substituted α-diazoacetamides such as 4-N3C6H4NHCOCHN2 (I) and 4,2-N3(HO)C6H3NHCOCHN2 to olefins and alcs. using either Rh(OMe)2 or preferably Rh(O2CCMe3)2 provided cyclopropanecarboxamides, e.g., II, and α-alkoxyacetamides, e.g., III, resp., without disrupting the azide functionality. Thus, 4-H2NC6H4NH2 was treated with HO2CCH2NHCO2CMe3 and DCC in THF to give 4-H2NC6H4NHCOCH2NHCO2CMe3 which was treated with NaNO2 and HCl in aqueous THF, and then NaN3 to give 4-N3C6H4NHCOCH2NHCO2CMe3. Deprotection of the latter compound with HCl-AcOH and then treatment with NaNO2 and AcOH in a mixture of THF, AcOEt and H2O gave 69% I. Treating I with (E)-PhCH:CHPh in the presence of Rh(O2CCMe3)2 in MeOCH2CH2OMe gave 30% II, whereas, similar treatment of I with cyclohexanol in the presence of Rh(O2CCMe3)2 gave 59% III. Azide-bearing α-diazo amides are potentially useful in the preparation of photoaffinity crosslinking reagents for studying the mechanism of action of natural products.

IT 17202-89-0P 105311-14-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 17202-89-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-phenyl- (CA INDEX NAME)

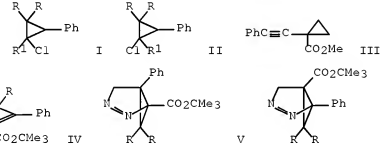



RN 105311-14-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-(4-azidophenyl)- (CA INDEX NAME)



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L25 ANSWER 10 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1983:612236 HCAPLUS Full-text
DOCUMENT NUMBER: 99:212236
ORIGINAL REFERENCE NO.: 99:32651a,32654a
TITLE: Synthesis and addition reactions of 2-phenyl-1-cyclopropene-1-carboxylates
AUTHOR(S): Norden, Wolfgang; Sander, Volker; Weyerstahl, Peter
CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ. Berlin, Berlin, D-1000, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1983), 116(9), 3097-111
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 99:212236
ED Entered STN: 12 May 1984
GI

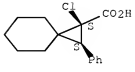


AB RRC:CHPh [R = Me, Ph; RR = (CH2)n (n = 3-6)] were converted into cyclopropanecarboxylic acids I and II (R1 = CO2H) via I (R1 = Cl). Spiropentane I [RR = (CH2)2, R1 = Cl] gave ethynylcyclopropane III via anionic ring cleavage with BuLi. I and II (R = CO2CMe3) gave cyclopropenes IV, but the trans isomers I reacted much faster than cis isomers II. C-3 unsubstituted chlorocyclopropanecarboxylates do not give stable cyclopropene esters even with Li dialkylamides. Addition reactions of CH2N2, thiophenolate, malonate, and CH2(CN)2 with IV were studied. Thus, e.g., IV and CH2N2 gave bicyclic pyrazolines V and VI.

IT 87957-51-5P

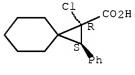
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with isobutene)
RN 87957-51-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-chloro-2-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



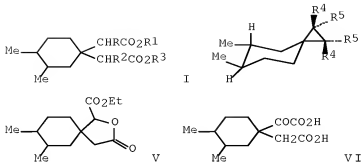

IT 87957-52-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87957-52-6 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-chloro-2-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.




OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L25 ANSWER 11 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1980:549871 HCAPLUS Full-text
DOCUMENT NUMBER: 93:149871
ORIGINAL REFERENCE NO.: 93:23879a,23882a
TITLE: Studies in the cyclohexane series. Part XX. Study on the products of hydrolysis of mono- and dibromo esters of 3,4-dimethylcyclohexane-1,1-diacetic acid
AUTHOR(S): Gautam, R. K.; Saharia, G. S.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110007, India
SOURCE: Journal of the Institution of Chemists (India) (1978), 50(6), 259-63
CODEN: JOICA7; ISSN: 0020-3254
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:149871
ED Entered STN: 12 May 1984
GI

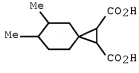


AB Cyclohexanediacetates I [R = R1 = H, R2 = Br, R3 = Et (II); R = R2 = Br, R1 = R3 = Et (III)] were prepared and their hydrolysis products were examined Thus, refluxing the anhydride of I (R = R3 = H) in EtOH gave I (R = R2 = H, R3 = Et) which was monobrominated by Br-PCl5 to give 65% II. Hydrolysis of II by KOH gave IV (R4 = H, R5 = CO2H; R4 = CO2H, R5 = H) and V. and V. Bromination of I (R = R3 = H) by Br gave I (R = R2 = Br, R1 = R3 = H). Esterification of this dibromo acid with EtOH gave III. III was hydrolyzed by refluxing with KOH to give VI.

IT 74281-66-6P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, during hydrolysis of cyclohexanebromodiacetate)

RN 74281-66-6 HCAPLUS

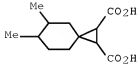
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 5,6-dimethyl-, stereoisomer (CA INDEX NAME)



IT 74244-35-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 74244-35-2 HCAPLUS

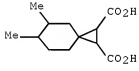
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 5,6-dimethyl-, stereoisomer (CA INDEX NAME)



IT 74282-01-2P 74310-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 74282-01-2 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 5,6-dimethyl-, stereoisomer, compd. with phenylmethyl carbamimidothioate (9CI) (CA INDEX NAME)

CM 1

CRN 74244-35-2
CMF C12 H18 O4



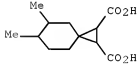
CM 2

CRN 621-85-2
CMF C8 H10 N2 S

RN 74310-28-4 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 5,6-dimethyl-, stereoisomer, compd. with phenylmethyl carbamimidothioate (9CI) (CA INDEX NAME)

CM 1

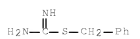
CRN 74281-66-6
CMF C12 H18 O4



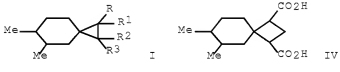
CM 2

CRN 621-85-2

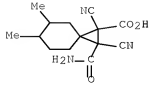
CMF C8 H10 N2 S



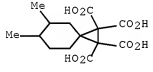
L25 ANSWER 12 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1980:75937 HCAPLUS Full-text
DOCUMENT NUMBER: 92:75937
ORIGINAL REFERENCE NO.: 92:12499a,12502a
TITLE: Studies in the cyclohexane series. Part XXI. Synthesis of 5,6-dimethylspiro[2.5]octane-1,2- and 6,7-dimethylspiro[3.5]nonane-1,3-dicarboxylic acids
AUTHOR(S): Gautam, R. K.; Saharia, G. S.
CORPORATE SOURCE: Dep. Chem., Univ. Delhi, Delhi, 110007, India
SOURCE: Journal of the Institution of Chemists (India) (1979), 51(1), 25-8
CODEN: JOICA7; ISSN: 0020-3254
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 92:75937
ED Entered STN: 12 May 1984
GI



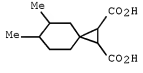
AB 5,6-Dimethylspiro[2.5]octane-1,2-dicarboxylic acid (I; R = R3 = H, R1 = R2 = CO2H) (II) was prepared by brominating α,α1-dicyano-3,4-dimethyl-1,1-cyclohexanediacetic acid imide (III) followed by treatment with HCO2H to give I (R = R3 = CN, R1R2 = CONHCO), which was hydrolyzed and the tetracarboxylic acid was partially decarboxylated to give cis-II. Cyclization of III with CH2I2 followed by similar hydrolysis and decarboxylation gave cis-IV.
IT 72612-65-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 72612-65-8 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-(aminocarbonyl)-1,2-dicyano-5,6-dimethyl- (CA INDEX NAME)



IT 72612-66-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and partial decarboxylation of)
RN 72612-66-9 HCAPLUS
CN Spiro[2.5]octane-1,1,2,2-tetracarboxylic acid, 5,6-dimethyl- (CA INDEX NAME)

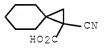


IT 72612-67-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72612-67-0 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 5,6-dimethyl- (CA INDEX NAME)



L25 ANSWER 13 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1979:137315 HCAPLUS Full-text
DOCUMENT NUMBER: 90:137315
ORIGINAL REFERENCE NO.: 90:21757a,21760a
TITLE: An improved procedure for the homologation of cycloalkanones
AUTHOR(S): Saunier, Yves Marie; Danion-Bougot, Renee; Danion, Daniel; Carrie, Robert
CORPORATE SOURCE: Groupe Rech. Physicochim. Struct., Univ. Rennes, Rennes, Fr.
SOURCE: Journal of Chemical Research, Synopses (1978), (11), 436-7
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal

LANGUAGE: English/French
OTHER SOURCE(S): CASREACT 90:137315
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Treating cycloalkylidenecyanoacetates I (n = 4, 5, 6, 7, 11), available through Cope-Knoevenagel condensations from cycloalkanones, with diazomethane at -20° followed by thermolysis of the resulting pyrazolines gave I (n = 5, 6, 7, 8, 12, resp.). The latter compds. could either be further ring enlarged or hydrolyzed to give the corresponding cycloalkanones. Overall yields of cycloalkanone for a single ring enlargement were as high as 76%; and for an enlargement by 2 or 3 C atoms, yields of up to 72% were obtained. 2-Methylcyclotetradecanone, readily available by this procedure, is a very convenient precursor of muscone.
IT 69586-12-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 69586-12-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1-cyano- (CA INDEX NAME)




OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L25 ANSWER 14 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1978:597047 HCAPLUS Full-text
DOCUMENT NUMBER: 89:197047
ORIGINAL REFERENCE NO.: 89:30615a,30618a
TITLE: Racemic disubstituted alkyl cis- and trans-3-formylcyclopropane-1-carboxylates
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | | DATE | |
|---|---|---|---|---|---|---|
| JP 53084947 | A | 19780726 | JP 1977-157521 | | 19771228 | <-- |
| JP 62003141 | B | 19870123 | | | | |
| FR 2376120 | A1 | 19780728 | FR 1976-39533 | | 19761230 | <-- |
| FR 2376120 | B1 | 19801003 | | | | |
| BE 862461 | A1 | 19780629 | BE 1977-183959 | | 19771229 | <-- |
| GB 1596030 | A | 19810819 | GB 1977-54178 | | 19771229 | <-- |
| CH 627149 | A5 | 19811231 | CH 1977-16306 | | 19771230 | <-- |
| CH 627731 | A5 | 19820129 | CH 1981-2798 | | 19810429 | <-- |
| JP 61171453 | A | 19860802 | JP 1985-258818 | | 19851120 | <-- |
| PRIORITY APPLN. INFO.: | | | FR 1976-39533 | A | 19761230 | <-- |
| | | | CH 1977-16306 | A | 19771230 | <-- |

OTHER SOURCE(S): CASREACT 89:197047; MARPAT 89:197047
ED Entered STN: 12 May 1984
GI

I

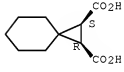
AB Racemic esters (I; R,R1 = C1-16 alkyl, RR1 = C3-7 alkylene; R2 = C1-6 alkyl; R3 = CHO) were prepared by reduction of half esters (I; R, R1, R2 as above; R3 = CO2H) followed by oxidation of the hydroxymethyl derivs. (I; R, R1, R2 as above, R3 = CH2OH). Thus, 0.001 mol trans-I (R = R1 = Me, R2 = Et, R3 = CO2H) was reduced with 0.004 mol B2H6 in THF under N to give 70% trans-I (R = R1 = Me, R2 = Et, R3 = CH2OH), which (0.001 mol) was oxidized by 0.0015 mol CrO3-pyridine complex under N to give 66% trans-I (R = R1 = Me, R2 = Et, R3 = CHO). Similarly prepared were 3 addnl. trans-I [R3 = CHO: RR1 = (CH2)5, R2 = Me; RR1 = (CH2)6, R2 = Et; R = R1 = R2 = Et].

IT 68194-50-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)

RN 68194-50-3 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

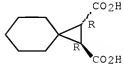


IT 67911-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and isomerization of)

RN 67911-20-0 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, trans- (9CI) (CA INDEX NAME)

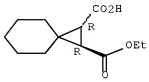
Relative stereochemistry.



IT 67911-12-0 67911-27-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)

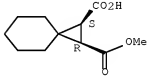
RN 67911-12-0 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, monoethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



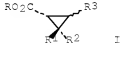

RN 67911-27-7 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, monomethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.




OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L25 ANSWER 15 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1978:579565 HCAPLUS Full-text
DOCUMENT NUMBER: 89:179565
ORIGINAL REFERENCE NO.: 89:27878h,27879a
TITLE: New stereospecific synthesis of cis and trans d,l-chrysanthemic esters and analogs via a common intermediate
AUTHOR(S): Devos, M. J.; Denis, J. N.; Krief, A.
CORPORATE SOURCE: Dep. Chem., Univ. Namur, Namur, Belg.
SOURCE: Tetrahedron Letters (1978), (21), 1847-50
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
GI



I

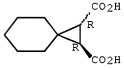
AB The hemicaronic aldehydes I [R = Et, R1 = R2 = Me, Et, R1R2 = (CH2)5; R = Me, R1R2 = (CH2)4] (R3 = β-CHO) and I [R = Me, R1 = R2 = Me, Et, R1R2 = (CH2)5] (R3 = α-CHO), known precursors of trans and cis chrysanthemic esters and analogs, were prepared stereospecifically from cis- or trans-RO2CCH:CHCO2R, initially by reaction with Ph3P+C-R1R2 to give I (R3 = β-CO2R). The latter were converted to trans aldehydes by sequential treatment with KOH-ROH, B2H6.THF, and CrO3-pyridine. The I (R3 = β-CO2R) were converted to cis aldehydes by sequential treatment with KOH-ROH, Ac2O, MeOH-pyridine, B2H6.THF, and CrO3-pyridine.

IT 67911-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of, anhydride from)

RN 67911-20-0 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

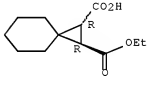



IT 67911-12-0P 67911-27-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and diborane reduction of)

RN 67911-12-0 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, monoethyl ester, trans- (9CI) (CA INDEX NAME)

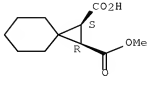
Relative stereochemistry.




RN 67911-27-7 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, monomethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 6 THERE ARE 6 CAPLUS RECORDS THAT CITE THIS RECORD (6 CITINGS)

L25 ANSWER 16 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1977:170935 HCAPLUS Full-text
DOCUMENT NUMBER: 86:170935
ORIGINAL REFERENCE NO.: 86:26837a,26840a
TITLE: Cyclopropanecarboxylic acids and esters
INVENTOR(S): Martel, Jacques; Huynh, Chanh; Buendia, Jean
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.
SOURCE: U.S., 22 pp. Division of U.S. 3,786,052.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| US 3997586 | A | 19761214 | US 1973-395146 | 19730907 <-- |
| US 3786052 | A | 19740115 | US 1971-168441 | 19710802 <-- |
| US 4206140 | A | 19800603 | US 1978-910695 | 19780530 <-- |
| PRIORITY APPLN. INFO.: | | | US 1967-662278 | A2 19670822 <-- |
| | | | US 1969-879942 | A2 19691125 <-- |
| | | | US 1971-168441 | A3 19710802 <-- |
| | | | FR 1966-74404 | A 19660826 <-- |
| | | | FR 1966-74405 | A 19660826 <-- |
| | | | FR 1967-96425 | A 19670224 <-- |
| | | | FR 1967-110719 | A 19670616 <-- |
| | | | FR 1967-114833 | 19670719 <-- |
| | | | FR 1968-175375 | A 19681126 <-- |
| | | | US 1973-395146 | A3 19730907 <-- |
| | | | US 1976-749402 | A3 19761210 <-- |

ED Entered STN: 12 May 1984
GI

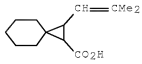

I

AB About 20 carboxylates [I, Z = Et2C, (Me2CHCH2)2C, Ph2C, cyclpentylidene, cyclohexylidene, Pr2C, EtCHMeCH(CHMe2), etc.; R = 5-benzyl-2-furylmethyl, 3-(2-cyclohexen-1-yl)-2-methyl-4-oxo-2-cyclopenten-1-yl, residue of allethrolone or cinerolone], useful as insecticides (no data), were prepared, e.g., by treating the appropriate carboxylic acid chlorides with alcs. Thus, I (Z = Et2C, R = Et), obtained by condensation of Et2C:CHCH2SO2Ph with Me2C:CHCO2Et, was hydrolyzed and the acid esterified with allethrolone to give I (Z = Et2C, R = allethrolone residue).

IT 26069-11-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acid chloride formation of)

RN 26069-11-4 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 2-(2-methyl-1-propen-1-yl)- (CA INDEX NAME)




OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L25 ANSWER 17 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1975:527541 HCAPLUS Full-text
DOCUMENT NUMBER: 83:127541
ORIGINAL REFERENCE NO.: 83:20019a,20022a
TITLE: Pesticide composition containing cyclopropane carboxylates
PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V., Neth.
SOURCE: Neth. Appl., 15 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE | |
|---|---|---|---|---|---|
| NL 7413166 | A | 19750410 | NL 1974-13166 | 19741007 | <-- |
| CA 1052797 | A1 | 19790417 | CA 1974-208231 | 19740830 | <-- |
| BE 820418 | A2 | 19750327 | BE 1974-1006199 | 19740927 | <-- |
| US 3950535 | A | 19760413 | US 1974-510197 | 19740930 | <-- |
| DD 115841 | A5 | 19751020 | DD 1974-181521 | 19741004 | <-- |
| AU 7474004 | A | 19760408 | AU 1974-74004 | 19741004 | <-- |
| FR 2246533 | A1 | 19750502 | FR 1974-33630 | 19741007 | <-- |
| FR 2246533 | B1 | 19780324 | | | |
| JP 50062957 | A | 19750529 | JP 1974-114789 | 19741007 | <-- |
| JP 58021885 | B | 19830504 | | | |
| DE 2447735 | A1 | 19750821 | DE 1974-2447735 | 19741007 | <-- |
| ZA 7406362 | A | 19751126 | ZA 1974-6362 | 19741007 | <-- |
| BR 7408318 | A | 19760427 | BR 1974-8318 | 19741007 | <-- |
| GB 1437987 | A | 19760603 | GB 1973-46926 | 19741007 | <-- |
| HU 172534 | B | 19780928 | HU 1974-SE1747 | 19741007 | <-- |
| CH 608170 | A5 | 19781229 | CH 1974-13441 | 19741007 | <-- |
| US 4021466 | A | 19770503 | US 1975-607396 | 19750825 | <-- |
| PRIORITY APPLN. INFO.: | | | GB 1973-46926 A | 19731008 | <-- |
| | | | US 1974-510197 A3 | 19740930 | <-- |

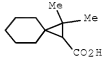
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB Insecticidal and acaricidal spirocyclopropanecarboxylates were prepared with the general formula I (R = R1 = alkyl; R2 = H, alkynyl, or CN; R3 = aromatic or heterocyclic group; n = 2-5). For example, 5-benzylfur-3-ylmethyl 2,2-dimethyl-3- spiro(cyclobutane)cyclopropanecarboxylate (II) [56338-11-5], applied as a 0.7% suspension to leaves of host plants, was totally effective against spider mites (Tetranychus urticae), cabbageworms (Pieris brassicae),

and aphids (Megoura viciae) and partially effective against leaf beetles (Phaedon cochleariae). II was also effective against house flies when applied topically (1 µl of a 1.0% solution). II was prepared from the corresponding acid by conversion to the acid chloride and reaction with 2-benzyl-4-hydroxymethylfuran [20416-09-5] in the presence of Et3N.

IT 55109-24-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with arylalkyl bromides)

RN 55109-24-5 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 2,2-dimethyl- (CA INDEX NAME)




L25 ANSWER 18 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1975:86117 HCAPLUS Full-text

DOCUMENT NUMBER: 82:86117

ORIGINAL REFERENCE NO.: 82:13763a,13766a

TITLE: 1-Halocyclobutan-2-ones

INVENTOR(S): Boyce, Clive B. C.; Searle, Robert J. G.; Davis, Royston Henry

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij B. V.

SOURCE: Ger. Offen., 11 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 2417615 | A1 | 19741107 | DE 1974-2417615 | 19740410 <-- |
| IT 1005785 | B | 19760930 | IT 1974-42674 | 19740405 <-- |
| BE 813520 | A1 | 19741010 | BE 1974-1005867 | 19740410 <-- |
| FR 2225407 | A1 | 19741108 | FR 1974-12630 | 19740410 <-- |
| BR 7402924 | D0 | 19741119 | BR 1974-2924 | 19740410 <-- |
| JP 50030846 | A | 19750327 | JP 1974-40129 | 19740410 <-- |
| JP 58010371 | B | 19830225 | | |
| DD 113347 | A5 | 19750612 | DD 1974-177810 | 19740410 <-- |
| HU 168443 | B | 19760428 | HU 1974-SE1720 | 19740410 <-- |
| SU 554809 | A3 | 19770415 | SU 1974-2014993 | 19740410 <-- |
| CH 589584 | A5 | 19770715 | CH 1974-5024 | 19740410 <-- |
| NL 7404949 | A | 19741018 | NL 1974-4949 | 19740411 <-- |
| NL 189756 | B | 19930216 | | |
| NL 189756 | C | 19930716 | | |
| GB 1437832 | A | 19760603 | GB 1973-18195 | 19740411 <-- |

PRIORITY APPLN. INFO.: GB 1973-18195 A 19730416 <--

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

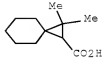
AB Eight cyclobutanones I [R = Me; R1 = Me, Pr, Me2C:-CH, or Ph; or RR1 = (CH2)2, (CH2)3, or (CH2)5; R2 = H or Me; R3 = Cl or Br], used for the preparation of the cyclopropanecarboxylic acids II, were prepared by halogenation of I (R3 =

H). Thus, I (R = Me, R1 = Me2C:CH, R2 = R3 = H) was treated with SO2Cl2 in CHCl3 at 20° to give I (R = Me, R1 = Me2C:CH, R2 = H, R3 = Cl). Treatment of I (R = R1 = Me, R2 = R3 = H) with Br in CHCl3 gave I (R = R1 = Me, R2 = H, R3 = Br), which on refluxing in aqueous Na2CO3 gave II (R = R1 = Me, R2 = H).

IT 55109-24-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 55109-24-5 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 2,2-dimethyl- (CA INDEX NAME)




OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

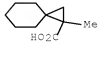
L25 ANSWER 19 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1974:14632 HCAPLUS Full-text
DOCUMENT NUMBER: 80:14632
ORIGINAL REFERENCE NO.: 80:2457a,2460a
TITLE: Halogenated ketenes. XXIV. Cycloaddition of alkylhaloketenes and methylenecycloalkanes. Spiro compounds
AUTHOR(S): Brady, William T.; Patel, Arvind D.
CORPORATE SOURCE: Dep. Chem., North Texas State Univ., Denton, TX, USA
SOURCE: Journal of Organic Chemistry (1973), 38(24), 4106-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 80:14632
ED Entered STN: 12 May 1984

AB The cycloaddn. of methylchloroketene with methylenecyclohexane, methylenecyclobutane, β-pinene and 5-methylene-2-norbornene to yield the corresponding spiro[3.5] and spiro[3.3] ketones was investigated. The cycloaddn. of ethylchloroketene with methylenecyclobutane was also described. The spiro ketones were reduced to the corresponding spiro alcohols. Some base-catalyzed rearrangement reactions were described, including ring contractions to spiro[5.2] compounds.

IT 42077-50-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

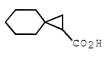
RN 42077-50-9 HCAPLUS

CN Spiro[2.5]octane-1-carboxylic acid, 1-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

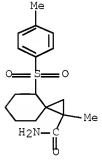
L25 ANSWER 20 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1972:413889 HCAPLUS Full-text
DOCUMENT NUMBER: 77:13889
ORIGINAL REFERENCE NO.: 77:2298h,2299a
TITLE: exo-Bicyclo[3.1.0]hexane-6-carboxylic acid and related compounds, oral hypoglycemic agents
AUTHOR(S): Rynbrandt, Ronald H.; Dutton, Fred E.; Schmidt, Fredericka L.
CORPORATE SOURCE: Diabetes Res., Upjohn Co., Kalamazoo, MI, USA
SOURCE: Journal of Medicinal Chemistry (1972), 15(4), 424-6
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984
AB Exo-bicyclo[3.1.0]hexane-6-carboxylic acid (I) [4971-24-8] had good hypoglycemic activity at 6.25 mg/kg in glucose-primed, fasted intact rat. A number of related compds. were prepared by known methods to determine the various structural features necessary for hypoglycemic activity. The bicyclic ring system in I appears to be necessary for activity in that cyclopropanecarboxylic acid [1759-53-1] and cyclohexanecarboxylic acid [98-89-5] were both inactive. The exo configuration is required in that endo-bicyclo[3.1.0]hexane-6-carboxylic acid [34898-25-4] was inactive. Variations in the ring size gave exo-bicyclo[4.1.0]heptane-7-carboxylic acid (IIe [21448-77-1], which possessed greater activity than I (2.0 mg/kg being the lowest dose that consistently produced a hypoglycemic response). Larger ring compds. (III and IV), a spirocyclopropane analog (V) and a tricyclic analog had little or no activity. Exo-bicyclo[3.1.0]hexane-6-acetic acid (VII) [34898-27-6] had good activity (12.5 mg/kg), as did all esters (VIII) and primary and secondary amides (IX) of I.
IT 17202-86-7
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(hypoglycemic activity of)
RN 17202-86-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid (CA INDEX NAME)



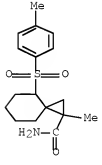

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L25 ANSWER 21 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1972:25160 HCAPLUS Full-text
DOCUMENT NUMBER: 76:25160
ORIGINAL REFERENCE NO.: 76:4087a,4090a
TITLE: Reaction of tosylazocyclohexene with dienophiles
AUTHOR(S): Barbieri, W.; Bernardi, L.; Masi, P.; Vigevani, A.; Caglioti, L.; Rosini, G.
CORPORATE SOURCE: Ist. Ric., Farmitalia, Milan, Italy
SOURCE: Tetrahedron (1971), 27(22), 5505-13

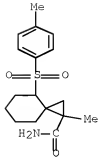
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 76:25160
ED Entered STN: 12 May 1984
AB The stereochemistry of the 1:1 adducts of tosylazocyclohex-1-ene with various dienophiles (Δ1-pyrazolines) is discussed on the basis of chemical and physicochem. evidence. The structure of the Δ2-pyrazolines and the spirocyclopropanes arising from the adducts, is also discussed.
IT 34706-07-5P 34709-10-9P 34709-11-0P
34709-12-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 34706-07-5 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-4-[(4-methylphenyl)sulfonyl]-, [1α,3β(S*)]- (9CI) (CA INDEX NAME)



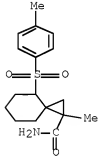

RN 34709-10-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-4-[(4-methylphenyl)sulfonyl]-, [1α,3α(S*)]- (9CI) (CA INDEX NAME)




RN 34709-11-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-4-[(4-methylphenyl)sulfonyl]-, [1α,3α(R*)]- (9CI) (CA INDEX NAME)



RN 34709-12-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, 1-methyl-4-[(4-methylphenyl)sulfonyl]-, [1α,3β(R*)]- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L25 ANSWER 22 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1970:100135 HCAPLUS Full-text
DOCUMENT NUMBER: 72:100135
ORIGINAL REFERENCE NO.: 72:18137a,18140a
TITLE: dl-Allethrolone esters of cyclopropanecarboxylic acids
INVENTOR(S): Martel, Jacques; Huynh Chanh
PATENT ASSIGNEE(S): Roussel-UCLAF
SOURCE: Fr., 8 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 6
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| FR 1507192 | A1 | 19671229 | FR 1966-74404 | 19660826 <-- |
| FR 1527844 | A1 | 19680607 | FR 1967-96425 | 19670224 <-- |
| BE 702662 | A | 19680214 | BE 1967-702662 | 19670814 <-- |
| CH 491071 | A | 19700531 | CH 1967-491071 | 19670815 <-- |

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|---|---|---|---|---|
| CH 491851 | A | 19700615 | CH 1967-491851 | 19670815 <-- |
| CH 509961 | A | 19710715 | CH 1969-18431 | 19670815 <-- |
| IL 28541 | A | 19751125 | IL 1967-28541 | 19670822 <-- |
| IL 38182 | A | 19751125 | IL 1967-38182 | 19670822 <-- |
| SE 369517 | B | 19740902 | SE 1967-11921 | 19670825 <-- |
| DE 1793721 | B2 | 19761223 | DE 1967-1793721 | 19670825 <-- |
| DE 1793721 | C3 | 19770825 | | |
| SE 391330 | B | 19770214 | SE 1971-133 | 19670825 <-- |
| DK 140720 | B | 19791105 | DK 1967-4303 | 19670825 <-- |
| DK 140720 | C | 19800421 | | |
| SU 691076 | A3 | 19791005 | SU 1967-1182999 | 19670826 <-- |
| NL 6711770 | A | 19680227 | NL 1967-11770 | 19670828 <-- |
| NL 162060 | B | 19791115 | | |
| NL 162060 | C | 19800415 | | |
| AT 287671 | B | 19710210 | AT 1967-7899 | 19670828 <-- |
| GB 1207371 | A | 19700930 | GB 1967-1207371 | 19670829 <-- |
| GB 1207372 | A | 19700930 | GB 1967-1207372 | 19670829 <-- |
| DK 131538 | B | 19750804 | DK 1970-6573 | 19701228 <-- |
| DK 133579 | B | 19760614 | DK 1970-6572 | 19701228 <-- |
| US 3786052 | A | 19740115 | US 1971-168441 | 19710802 <-- |
| US 4206140 | A | 19800603 | US 1978-910695 | 19780530 <-- |
| NL 7906529 | A | 19800131 | NL 1979-6529 | 19790830 <-- |
| NL 172853 | B | 19830601 | | |
| NL 172853 | C | 19831101 | | |
| PRIORITY APPLN. INFO.: | | | FR 1967-96425 | 19670224 <-- |
| | | | FR 1966-74405 | 19660826 <-- |
| | | | FR 1966-74404 A | 19660826 <-- |
| | | | FR 1967-110719 A | 19670616 <-- |
| | | | FR 1967-114833 A | 19670719 <-- |
| | | | FR 1967-114883 A | 19670719 <-- |
| | | | US 1967-662278 A2 | 19670822 <-- |
| | | | DK 1967-4303 A | 19670825 <-- |
| | | | NL 1967-11770 | 19670828 <-- |
| | | | FR 1968-175375 A | 19681126 <-- |
| | | | US 1969-879942 A | 19691125 <-- |
| | | | US 1971-168441 A3 | 19710802 <-- |
| | | | US 1973-395146 A3 | 19730907 <-- |
| | | | US 1976-749402 A3 | 19761210 <-- |

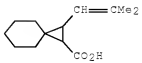
ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB The Et esters of the title acids [I, R1 = H or Pr, R2 = Me, Pr, or Pr, or (R1R2 =) (CH2)4-5] are prepared from esters (II) and sulfones Me2C:CHCH2SO2R3 (R3 = aryl) (III) and tert-BuOK (IV). The acids, as their acid chlorides, are esterified with dl-allethrolone. Thus, III (R3 = Ph) 12.9, II (R1 = H, R2 = Ph) 16.2, IV 13.82 g, and Me2SO 125 cm3 30 min at 20° gave 5.15 g Et ester of I (R1 = H, R2 = Ph) which was hydrolyzed to give I (R1 = H, R2 = Ph), m. 104°. Similarly were prepared Et esters of I (R1 = H, R2 = Me), b0.2 52°, n25D 1.462; I (R1 = R2 = Pr), b0.5 90-2°, n17D 1.4660; and I [(R1R2 =)(CH2)5], b0.7 93-7°. These esters were hydrolyzed to give I (R1 = H, R2 = Me), b0.07 81-2°, n25D 1.4820 (S-benzylthiuronium salt m. 194°), I (R1 = R2 = Pr), b0.1 116°, n23D 1.4760, and I [(R1R2 =)(CH2)5], m. 80° (isooctane); p-bromophenacyl ester m. 85°. I and SOCl2 gave the following acid chlorides I (CO2H = COCl): I (R1 = H, R2 = Ph), b0.3 101-3°, n23D 1.5522; I (R1 = H, R2 = Me), b0.8 51°; I (R1 = R2 = Pr), b0.1 80-5°, n23D 1.4819; I [(R1R2 =)(CH2)5], b0.2 78-80°, n25D 1.5080. The acid chloride of I (R1 = H, R2 = Ph) (1.742 g), 1.1126 g dl-allethrolone, 0.8 cm3 C5H5N, and 10 cm3 C6H6 gave an ester which was passed in C6H6 down an Al2O3 column to give 2.150 g ester, n24D 1.5487. Similarly the dl-allethrolone esters of I (R1 and R2 given) were prepd: H, Me, b0.01 127°; Pr, Pr; (R1 R2 =) (CH2)5, n25D 1.5193.

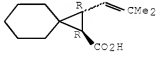
IT 26069-11-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26069-11-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-(2-methyl-1-propen-1-yl)- (CA INDEX NAME)



L25 ANSWER 23 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1969:460791 HCAPLUS Full-text
DOCUMENT NUMBER: 71:60791
ORIGINAL REFERENCE NO.: 71:11159a,11162a
TITLE: Synthesis of trans-chrysanthemic acid analogs
AUTHOR(S): Velluz, Leon; Nomine, Gerard; Martel, Jacques
CORPORATE SOURCE: Cent. Rech., Roussel-Uclaf, Romainville, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1969), 268(25), 2199-203
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 12 May 1984
GI For diagram(s), see printed CA Issue.
AB trans-Cyclopropanecarboxylic acids I, where R, R1, R2, and R3 are H and alkyl and aryl groups, are prepared from RR1C:CHCO2Et and R2R3C:-CHCH2SO2Ar. The R and R1 (and R2 and R3) can be identical or different; acids I (R = R1 = Me), where CR2R3 is a sym. cycloalkylidene group, are also prepared
IT 23057-77-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23057-77-4 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 2-(2-methyl-1-propen-1-yl)-, (1R,2R)-rel- (CA INDEX NAME)

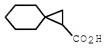
Relative stereochemistry.



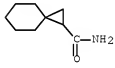
OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L25 ANSWER 24 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1969:3337 HCAPLUS Full-text
DOCUMENT NUMBER: 70:3337
ORIGINAL REFERENCE NO.: 70:593a,596a

TITLE: Reactions of sodium cyanide with 1,3-propanediol bistosylates. Influence of the intramolecular distance between the two reactions sites
AUTHOR(S): Seyden-Penne, Jacqueline; Roux-Schmitt, Marie Claude
CORPORATE SOURCE: C.N.R.S., Thiais, Fr.
SOURCE: Bulletin de la Societe Chimique de France ( 1968), (9), 3810-12
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
ED Entered STN: 12 May 1984
AB The reactions of NaCN with 1,1,-bis(hydroxymethyl)cycloalkanes (the cycloalkane contains 3-6 C) to give mixts. of 3,3-cycloalkyleneglutaronitriles and spiro-alkanecarbonitriles are described. The composition of the reactions product mixts. varies according to the intramol. distance between the 2 reactions sites.
IT 17202-86-7P 17202-88-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 17202-86-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid (CA INDEX NAME)




RN 17202-88-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide (CA INDEX NAME)



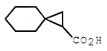

L25 ANSWER 25 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1968:505990 HCAPLUS Full-text
DOCUMENT NUMBER: 69:105990
ORIGINAL REFERENCE NO.: 69:19827a,19830a
TITLE: Chemistry of cyclopropanes. I. Synthesis and deamination of spiroamines
AUTHOR(S): Konzelman, L. M.; Conley, R. T.
CORPORATE SOURCE: Seton Hall Univ., South Orange, NJ, USA
SOURCE: Journal of Organic Chemistry (1968), 33(10), 3828-38
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

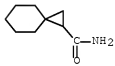
AB Four spirocyclopropylamines in which the adjacent spiro ring was varied from cyclopropyl to cyclohexyl were prepared and deaminated. 1-Aminospirohexane (I), 1-aminospiro[2.4]heptane (II), and 1-aminospiro[2.5]octane (III) were obtained by adding Et diazoacetate to the appropriate methylenecycloalkane, and converting the resulting spiro esters by hydrolysis and Curtius rearrangement into the corresponding spiro amines. Similarly, spiropentylamine (IV) was prepared from Et spiropentanecarboxylate. Deamination (aqueous HNO2-NaNO2) of I-III gave mixts. of unsatd. alcs. in which the adjacent cycloalkyl moiety remained intact. IV gave predominantly a mixture of 2- and 3-methylenecyclobutanols. These results are discussed in terms of the collapse or rearrangement of an initially formed spirocyclopropyl action.

IT 17202-86-7P 17202-88-9P 17202-89-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

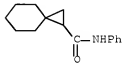
RN 17202-86-7 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid (CA INDEX NAME)



RN 17202-88-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide (CA INDEX NAME)



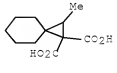
RN 17202-89-0 HCAPLUS
CN Spiro[2.5]octane-1-carboxamide, N-phenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 10 THERE ARE 10 CAPLUS RECORDS THAT CITE THIS RECORD (10 CITINGS)

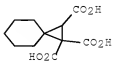
L25 ANSWER 26 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1965:58590 HCAPLUS Full-text
DOCUMENT NUMBER: 62:58590

ORIGINAL REFERENCE NO.: 62:10349a-e
TITLE: Cyclic acylals. XII. Synthesis of substituted cyclopropane-1,1-dicarboxylic acids
AUTHOR(S): Wessely, F.; Eitel, A.
CORPORATE SOURCE: Univ. Vienna
SOURCE: Monatshefte fuer Chemie (1964), 95(6), 1577-88
CODEN: MOCMB7; ISSN: 0026-9247
DOCUMENT TYPE: Journal
LANGUAGE: German
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 59, 6300e; 62, 6427e. Reactions of CH2N2 with substituted methylene-Meldrum's acids (I) gave a series of esters of spirocyclopropane-1,1-dicarboxylic acids (II) which were hydrolyzed to the corresponding acids (III). Some of the reactions with CH2N2 gave two products, one of which resulted from a ring expansion. The thin-layer chromatography of I is described. A suspension of I (n = 5) in MeOH was cooled to -70° and treated with CH2N2 in Et2O portionwise during 5 hrs. The excess CH2N2 and Et2O were removed in vacuo. The residue taken up in Et2O, filtered from any polymethylene formed, and then concentrated gave a residue (48%) which showed two m.ps., 93° and 105° (Et2O-petr. ether). Purification of this product by thin-layer chromatography gave 60% II(n = 5) and about 10% II (n = 6). A solution of I (n = 4) in MeOH was treated with CH2N2 to give 50% II (n = 5) which m. 93° and then partially solidified and gave another m.p. at 105°. II (n = 5) was hydrolyzed in alc. NaOH to give III (n = 5), m. 151°. Decarboxylation of III (n = 5) at 160-70° gave a lactone (IV), ν 1785 cm.-1; and an acid (V), m. 21-3°; Me ester ν 1740 cm.-1 (CCl4). Hydrogenation of V in the presence of Pd gave β-cyclohexylpropionic acid, m. 12°; amide m. 118°. I (n = 6), m. 55°, in MeOH was treated with CH2N2 to give II (n = 6), m. 101-3°. Similarly prepared was 2-cyclo-hexylcyclopropane-1,1-dicarboxylic acid, m. 163-6°. The following compds. were also prepared (type, R, R1, R2, and m.p.given): VI, Me, --, --, 79-80°; VII, Me, --, --, 148°; VI, CO2Et, --, --, 101°; VII, CO2H, --, --, 191-4°; VIII, Ph, Me, Me, --; VIII, Ph, H, CO2Et, 109-10°; VIII, PhCH-(CO2Et), H, CO2Et, 175°; VIII, Ph, H, Ph, --; VIII, Ph2CH, H, Ph, 175°.
IT 882-60-0P, Spiro[2.5]octane-1,1-dicarboxylic acid, 2-methyl-
944-07-0P, Spiro[2.5]octane-1,1-dicarboxylic acid
1021-30-3P, Spiro[2.5]octane-1,1,2-tricarboxylic acid
RL: PREP (Preparation)
(preparation of)
RN 882-60-0 HCAPLUS
CN Spiro[2.5]octane-1,1-dicarboxylic acid, 2-methyl- (CA INDEX NAME)




RN 944-07-0 HCAPLUS
CN Spiro[2.5]octane-1,1-dicarboxylic acid (CA INDEX NAME)

RN 1021-30-3 HCAPLUS
CN Spiro[2.5]octane-1,1,2-tricarboxylic acid (CA INDEX NAME)

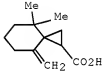


L25 ANSWER 27 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1963:403644 HCAPLUS Full-text
DOCUMENT NUMBER: 59:3644
ORIGINAL REFERENCE NO.: 59:666c-g
TITLE: Photochemical isomerization in the β-ionone series
AUTHOR(S): Mousseron-Canet, Magdeleine; Mousseron, Max; Legendre, Pierre; Wylde, James
CORPORATE SOURCE: Ecole Natl. Super Chim. Org., Brussels, Belg.
SOURCE: Bulletin de la Societe Chimique de France (1963) 379-83
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:3644
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 55, 27398b. The primary photochem. isomerization process was a trans → cis transformation; this very reactive intermediate was then converted to a conjugated exocyclic diene. Irradiation of 3 g. βcyclocitrylideneacetic acid (I) in 300 cc. hexane by a Hg-vapor lamp for 72 hrs. under N gave 800 mg. II and 1 g. III, m. 35-40°; S-benzylisothiuronium salt m. 162-4°. Irradiation of I in CH Cl3 or EtOH gave II, III, and IV. Irradiation of β-ionone gave V; semicarbazone m. 171-2°. III (1 g.) in 10 cc. anhydrous Et2O treated dropwise with stirring with 260 mg. MeLi in Et2O under N, and the mixture refluxed 2 hrs. gave 800 mg. V. α-Cyclocitrylideneacetic acid (200 mg.) (S-benzylisothiuronium salt m. 175°), obtained by the haloform reaction on α-ionone, on hydrogenation in 15 cc. HOAc with 100 mg. Adams PtO2 under atmospheric pressure gave VI (S-benzylthiuronium salt m. 165°), which was also obtained by a similar hydrogenation of III. An inconclusive preparation was made of VII (which might hypothetically be expected to be formed in the irradiation) by hydrogenation of IV to VIII, m. 54-5°, transformation of VIII by SOCl2 into the chloro ester, and dehalogenation by Na tert-amylate. Lactonization of 800 mg. III by 3.55 cc. HCO2H for 24 hrs. at room temperature gave chiefly II (with small amts. of IV); in the hot, the product was chiefly IV. A mixture of II and IV treated in the hot with alc. NaOH showed a considerable enrichment in IV. I (5 g.) in 100 cc. Et2O treated with CH2N2 in Et2O at 0° gave 95% IX, which on irradiation gave X. Saponification of X with

hot alc. KOH gave III. The mechanism of the irradiation reactions is discussed. The structures of many of the products were confirmed by ultraviolet and infrared measurements. The nuclear magnetic resonance spectra of vinylacetic acid, gem-dimethylcyclopropanecarboxylic acid, III, and VI were determined and compared.

IT 92904-33-1P, Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene- 95696-94-9P, Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene-, compound with 2-benzyl-2-thiopseudourea
RL: PREP (Preparation)
(preparation of)

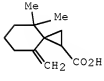
RN 92904-33-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene- (CA INDEX NAME)




RN 95696-94-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene-, compd. with phenylmethyl carbamimidothioate (1:1) (CA INDEX NAME)

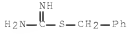
CM 1

CRN 92904-33-1
CMF C12 H18 O2



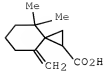

CM 2

CRN 621-85-2
CMF C8 H10 N2 S




OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

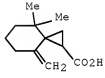
L25 ANSWER 28 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1963:403643 HCAPLUS Full-text
DOCUMENT NUMBER: 59:3643
ORIGINAL REFERENCE NO.: 59:665e-h,666b-c
TITLE: Stereochemical studies in the terpene series. II. Structure of the acid obtained by rearrangement of pinolic acid in acid medium
AUTHOR(S): Harispe, Marcelle; Mea, Dominique; Horeau, Alain; Jacques, Jean
CORPORATE SOURCE: Coll. France, Paris
SOURCE: Bulletin de la Societe Chimique de France ( 1963) 472-5
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB cf. CA 57, 15157g. The hydroxy acid previously obtained (loc. cit.) by treatment of (-)-pinolic acid with cold dilute H2SO4 was shown to be I on the basis of the following data. I (2 g.) in 8 cc. HOAc treated with a solution of 0.72 g. CrO3 in 0.7 cc. water, and the mixture kept overnight gave 1.77 g. II, m. 59° (petr. ether), [α]20D 4° (c 2, dioxane); Na salt, [α]20D 1.3° (c 5, H2O). II boiled several min. with 2N alc. KOH isomerized to the cis acid (III), m. 82° (petr. ether), [α]20D° 39° (c 2.5, dioxane); Na salt, [α]20D 43° (c 5, H2O). In alkaline solution an equilibrium mixture of 90- 92% of the salt of III and of 8-10% of the salt of II was formed. III was identical with the acid obtained in 18% overall yield by oxidation of (+)-fenchone with CrO3-HOAc-Ac2O at 15° for 1.5 hrs. to form 2,6-dioxofenchane, and by treatment of the latter (2.53 g.)for 1 hr. at 100° with 1.5 g. KOH in 20 cc. absolute alc.; the 2 acids gave identical Me esters, oximes (m. 165°), and semicarbazones, cubic crystals, m. 223° (MeOH). The infrared spectra of the 2 semicarbazones were identical. The assignments of configurations to carbons 1, 3, and 4 of I and to carbons 1 and 4 of II and III were made on the basis of their origin and of the following exptl. data. The method for determination of the configurations of secondary hydroxyls (CA 56, 7384f) by partial esterification with α-phenylbutyric anhydride when applied to (-)-pinolic acid and I gave the configurations indicated. The configuration of the 4-Me was based on a consideration of the reaction mechanism involved in the formation of I. Formulas II and III were in agreement with the results of hydrogenation expts. III was hydrogenated as the Na salt by Pt-Raney Ni in EtOH to form IV, m. 121.5° (petr. ether), [α]20D 23° (c 3, EtOH); Me ester (by CH2N2 method), n21D 1.4651. II was not hydrogenated by Adams Pt in HOAc. The configuration of IV was determined by the method of partial esterification. Some of the configurations previously assigned (CA 57, 9883h) are in error.
IT 92904-33-1P, Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene- 95696-94-9P, Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene-, compound with 2-benzyl-2-thiopseudourea
RL: PREP (Preparation)
(preparation of)
RN 92904-33-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene- (CA INDEX NAME)



RN 95696-94-9 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 4,4-dimethyl-8-methylene-, compd. with phenylmethyl carbamimidothioate (1:1) (CA INDEX NAME)

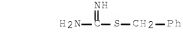
CM 1

CRN 92904-33-1
CMF C12 H18 O2



CM 2

CRN 621-85-2
CMF C8 H10 N2 S



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L25 ANSWER 29 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1963:8560 HCAPLUS Full-text
DOCUMENT NUMBER: 58:8560
ORIGINAL REFERENCE NO.: 58:1361g-h,1362a
TITLE: A study of the Thorpe-Ingold effect: the reaction of potassium hydroxide with a lactone of ethyl α-bromo-α'-hydroxy-1,1-cyclohexanediacetate
AUTHOR(S): Larson, H. O.; Sung, Gaylien S. K.
CORPORATE SOURCE: Univ. Hawaii, Honolulu
SOURCE: Australian Journal of Chemistry (1961), 15, 261-4
CODEN: AJCHAS; ISSN: 0004-9425
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

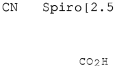
ED Entered STN: 22 Apr 2001

AB α,α'-Dihydroxy-1,1-cyclohexanediacetic acid (I) was produced in the title reaction and is thought to be the product regarded by Beesley, et al. (CA 9, 3059) as 1-hydroxy-trans-spiro[2,5]octane-1,2- dicarboxylic acid. Bromination of 50 g. 1,1-cyclohexanediacetic acid with PBr5 and Br (Thole and Thorpe CA 5, 2848) gave 22 g. liquid acid and 74 g. neutral product (II). Treatment of the acid with KOH gave 2.3 g. trans-spiro[2,5]-octanedicarboxylic acid, m. 238-9° (aqueous EtOH), λ 5.98 μ (KBr) (Ettlinger and Kennedy, CA 50, 8472h). Treatment of 54 g. II with pyridine gave 11.1 g. lactone (III) of Et α-bromo-α'-hydroxy-1,1-cyclohexanediacetate, m. 93.5-4.5° (C6H6), λ 5.62 and 5.73 μ (KBr). III (3.6 g.) and 3.6 g. KOH in 21 mL. H2O at 95-105° 20 min. gave 0.35 g. I, m. 215-17° (aqueous EtOH), λ 5.84 and 6.05 μ (KBr) or 5.74 and 5.82 μ (dioxane), NMR at 56.4, 64.4, and 1.52 cycles/s. (NaOD). III. (4.0 g.) and 22 g. 64% aqueous KOH at 140-50° 4 min. gave 0.30 g. Δ1-α-cyclohexylideneacetic acid, m. 90-1° (aqueous EtOH), λ 5.98 and 6.15 μ (KBr). The reactions of III are analogous to those of α,α'-dihydroxy-1,1-cyclopentanediacetic acid lactone (Becker and T., CA 15, 1018).

IT 90927-27-8P, Spiro[2.5]octane-1,2-dicarboxylic acid
RL: PREP (Preparation)
(preparation of)

RN 90927-27-8 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid (CA INDEX NAME)




L25 ANSWER 30 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1962:456434 HCAPLUS Full-text

DOCUMENT NUMBER: 57:56434

ORIGINAL REFERENCE NO.: 57:11242a-i,11243a-i,11244a-f

TITLE: Polyterpenes. IV. Oxidation products of thujopsene

AUTHOR(S): Nagahama, Shizuo; Kobayashi, Hiroshi; Akiyoshi, Saburo

CORPORATE SOURCE: Kyushu Univ., Fukuoka

SOURCE: Bulletin of the Chemical Society of Japan (1962), 35, 1140-5
CODEN: BCSJA8; ISSN: 0009-2673

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

ED Entered STN: 22 Apr 2001

GI For diagram(s), see printed CA Issue.

AB cf. ibid. 34, 1123(1961); CA 55, 2728c. Thujopsene (I) (shown to have structure Ia by Erdtman and Norin, CA 54, 24845e; Norin, CA 57, 7317d) gave a number of degradation products (CA 52, 10964a) on KMnO4 oxidation (in the present study on K2Cr2O7 oxidation) for which structural assignments were now made on the basis of the structure of I. I (100 g.) in 400 cc. ice-cold Me2CO oxidized with 250 g. finely powdered KMnO4 gave an oily or semisolid acid fraction, C15H22O4, which was treated with C6H6 [an acid (II) precipitated if it had been formed] and the C6H6 extract concentrated and cooled to give 10 g. oxo acid (III), C15H24O3, m. 165°, [α]D −120°; the mother liquor diluted with petr. ether and kept several weeks in a refrigerator gave an oxo acid (IV) and an oxo acid (IV); after collecting a 2nd and 3rd crop, the remaining IV was

converted to II, which was easily separated by treatment with alkali for 2-3 days. II, C15H22O4, m. 193° (decomposition), [α]D 21.6°, 4.5 g. obtained on KMnO4 oxidation of 100 g. I; IV, C15H22O4, m. 124°, [α]D -28.0°, 3.5 g. obtained from KMnO4 oxidation of 100 g. I; V, C14H22O3, m. 156°, [α]D -85.5°, 0.3 g. obtained from KMnO4 oxidation of 100 g. I. The neutral fraction (750 g., from several combined runs) fractionated in vacuo gave the following fractions: (1) 28.4% fraction, mainly unreacted I, containing a small amount of isomerized hydrocarbons, b11 .apprx.119-°, n23D 1.5030-1.5050, (2) 5.9% fraction, b11 119-30°, n23D 1.5057-1.5090, which was redistd., the fraction of maximum nD (1.6%, b6 95-100°, n23D 1.5097) chromatographed on Al2O3, and eluted with petr. ether to give 0.9% hydrocarbon, n30D 1.5111, d30 0.9245, [α]30D 40.4°, ν 1515 and 812 cm.-1 (further elution with C6H6 gave VI); (3) 5.8% fraction, b11 130-43°, n23D 1.5018-1.5030), which was redistd., the fraction of min. nD (1.5%, b20 125°, n23D 1.4987) chromatographed on Al2O3, and eluted with petr. ether to give a mixture of ketones [1 of these separated as semicarbazone, m. 205-6° (decomposition); from the mother liquor was obtained another impure semicarbazone, m. 201.5-2.5° (decomposition)] (further elution gave VI; C6H6 elution gave cedrol, m. 85.5-6.0°; elution with EtOAc followed by dilution of the eluate with petr. ether and cooling gave a ketone, C15H24O2, m. 116-17.5° (petr. ether), ν 3330 and 1740 cm.-1); (4) 18.2% fraction, b10 143-65°, n20D 1.5060-1.5100, which was chromatographed on Al2O3 and eluted to give (from a petr. ether-C6H6 eluate) 0.4% VII, (from an EtOAc eluate) 0.5% hydroxy ketone (VIII), C15H24O2, m. 68-70.5°, ν (Nujol) 3384, 3195, and 1702 cm.-1 [semicarbazone m. 214° (decomposition)], and (from an MeOH eluate) 1.4% lactone, C15H22O3, m. 81.5-2.5°, ν 1795 cm.-1; (5) 3.3% fraction, b10 165-80°, n15D 1.5178, which gave only 0.7% VII on similar treatment. Na2Cr2O7 (250 g.) in 750 g. AcOH added dropwise during 9 hrs. to 100 g. in 200 g. AcOH at 50-70° with stirring, the solution kept overnight, concentrated (250 g. AcOH removed), poured into 3 l. H2O, the product extracted with C6H6, separated into its acidic constituents, and this fraction treated as above gave 0.2 g. III, 0.4 g. II, 2.0 g. IV, and 4.0 g. V; the neutral fraction concentrated and distilled in vacuo gave 28 g. fraction, b11 140-6°, which deposited 4.1 g. VII (chromatography of the mother liquor gave 4.0 g. VII and 0.2 g. VIII). IV (280 mg.) in 15 cc. Me2CO treated with 420 mg. KMnO4 in 40 cc. Me2CO below 50° gave V, m. 154.5-6.0° (C6H6-petr. ether or EtOH-H2O). V (270 mg.) in 5 cc. AcOH treated with 500 mg. Na2Cr2O7 in 5 cc. AcOH, kept overnight (no color change observed), treated with 5 cc. dilute H2SO4, kept 2 days, the excess Na2Cr2O7 decomposed with EtOH, the mixture diluted with H2O, the product isolated with Et2O, and triturated with C6H6 gave 45 mg. IX, m. 183-5° (decomposition); from the C6H6 solution was isolated unchanged V. V (500 mg.) oxidized with a hypobromite solution gave 400 mg. CBr4; workup of the acid products gave 100 mg. IX. Treatment of IV with CH2N2 gave the Me ester of III, m. 85-7° (petr. ether), [α]17D -187° (c 0.593, EtOH), its infrared and ultraviolet spectra being consistent with structure X. In the solid state, IV appeared to exist as a lactone (ν 1761 cm.-1) and was therefore assigned structure XI. IV in 5% aqueous NaOH kept overnight at room temperature and acidified gave II. EtOH or Et2O solns. of IV containing HCl gave only unchanged IV. The unsatd. oxo acid XII was obtained by dehydration of II (loc. cit.). XII (2.55 g.), 2 cc. N2H4.H2O (XIII), 2.5 g. KOH, and 25 cc. O(CH2CH2OH)2 (XIV) refluxed 4 hrs., diluted with H2O, and acidified gave 1.54 g. XV, m. 171-2° (EtOH), [α]30D -21.2° (c 1.19, CHCl3). To 186 mg. XV in 4 cc. 3% aqueous KOH was added 10 cc. 2% aqueous KMnO4, stirred 1.5 hrs., acidified, and treated with NaHSO3 gave XII, m. 206° (EtOH-H2O). Hinokiic acid (XVI) (2.4 g.) in 20 cc. Me2CO treated 1.5 hrs. with 5.0 g. KMnO4 in Me2CO, evaporated, the residue extracted with Et2O, the Et2O solution extracted with aqueous NaHCO3, and evaporated gave 120 mg. XVII; the aqueous NaHCO3 extract yielded 200 mg. crude XVIII, m. 206-11° [the mother liquor treated with CH2N2, the product (1.3 g.) chromatographed on Al2O3, and eluted

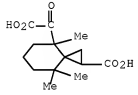
with 1:1 petr. ether-C6H6 gave 165 mg. di-Me ester of IX]. XVI (1.05 g.), 1.05 g. Cu powder, and 10 cc. quinoline heated 2 hrs. at 230-50°, filtered, the filtrate combined with distillate, diluted with Et2O, the solution washed with aqueous HCl, aqueous NaHCO3, and H2O, dried, evaporated, and the residual solid (320 mg.) distilled in vacuo gave XIX, m. 47° (MeOH), [α]30D -135° (c 0.933, EtOH.) Similar treatment of 1 g. XV gave XX, m. 12-14°, n17D 1.5042, [α]30D -114° (c 0.957, EtOH). Similar treatment of XII gave VII. VII (5 g.) treated with 3.3 cc. XIII, 4.8 g. KOH, and 50 cc. XIV and the resulting waxy product recrystd. several times from MeOH (with cooling in a dry ice-MeOH bath) gave 2.85 g. mixture of XIX and XX, m. 33-5°. To 550 mg. XIX in 10 cc. Me2CO was added 2 g. KMnO4 in 50 cc. Me2CO, the mixture stirred 1.5 hrs. below 40°, kept overnight, and worked up as usual to give 60 mg. XVIII, m. 210-11.5° (EtOH-H2O). Similar oxidation of 710 mg. XX gave 170 mg. IX. Alkaline KMnO4 oxidation of 290 mg. XII in the usual way gave (from the neutral fraction) 76 mg. XVII, m. 211-12° (petr. ether). KMnO4 (4.27 g.) in 100 cc. H2O added to VII, the mixture stirred 2.5 hrs. below 70°, and worked up as usual gave (from the acid fraction) 90 mg. IX and (from the neutral fraction) 165 mg. XVII, m. 206-7°. To 30 g. II in 450 cc. AcOH (incomplete solution) was added 12 g. Na2Cr2O7 in 50 cc. AcOH, the mixture kept 1 week at room temperature, the precipitate [7.84 g. II, m. 205.5-7.0° (decomposition)] filtered off, the filtrate concentrated to 1/3 its volume, poured into 1 l. H2O, the precipitate filtered off, and triturated with hot C6H6 to give 4.0 g. XXI, m. 218-21° (EtOH), [α]14D 272° (c 0.93, EtOH); the C6H6 solution extracted with aqueous NaHCO3 and evaporated gave a mixture of XII and XVII; acidification of the alkaline extract gave 440 mg. IX. With a ratio of 20 g. Na2Cr2O7/15 g. II the yield of XXI was diminished, but a larger amount (8 g.) of a mixture of XII and XVII was obtained. XXI (1.34 g.) in 40 cc. AcOH treated with 1.75 g. Na2Cr2O7 in 10 cc. AcOH, the mixture kept 5 hrs. below 50°, concentrated to 1/2 volume, diluted with H2O, the precipitate dissolved in C6H6, the solution freed from acids, and evaporated gave 960 mg. XXII, m. 179.5-80.0° (chromatography on Al2O3), mixed m.p. [with XXII prepared from VI, Kobayashi, et al., ibid. 34, 1123(1961)] 181-2.5°. IV was therefore assigned structure XXIII. Treatment of V with CH2N2 gave the Me ester (XXIV), m. 69-71°, [α]D -211° (c 0.78, EtOH). XXIV (140 mg.) refluxed 2 hrs. with 5% MeOH-NaOH, the solution poured into H2O, acidified, the product triturated with petr. ether, and recrystd. from Et-OH-H2O gave (from 1st crop) 5 mg. XXI, m. 219-20° (decomposition), and (from a 2nd crop) V. Treatment of V with Ac2O in pyridine gave XXV, m. 80.5-3.0° (EtOH). XXV (46 mg.) refluxed 1 hr. in 5 cc. 5% aqueous NaOH gave 12 mg. V. XXV (85 mg.) in MeOH-KOH refluxed 2 hrs., concentrated to 1/2 volume, poured into H2O, and the precipitate purified gave XXIV; acidification of the filtrate gave a small amount of XXI. V on the basis of spectral evidence and the preceding expts. existed as a pseudo acid and was assigned structure XXVI. IV (680 mg.) added to 20 cc. aqueous NaOBr, kept 2.5 hrs., treated with NaHSO3 and aqueous HCl, the resulting gel extracted with Et2O, and the extract evaporated gave XXVII (R = R' = H), m. 178-80° (decomposition), ν 3378, 1745, and 1667 cm.-1 Alternatively, the gel-product was treated overnight with alkaline H2O2, acidified, the precipitate dissolved in MeOH-H2O, and the solution deposited an oil, which solidified, ν (Nujol) 3333, 1727, and 1675 cm.-1, and then XXVII (R = R' = H), m. 178-80°, ν 3408, 3155, and 1721 cm.-1; with CH2N2 both products gave the same di-Me ester [XXVII (R = R' = Me)], m. 80.5-2.5°, which was identical with the di-Me ester obtained from the gel without treatment with H2O2. The different infrared spectra of the several samples of XXVII (R = R' = H) was attributed to the presence of varying proportions of XXVIII (R = H). XII (1.1 g.) ozonolyzed 3 hrs. in 80 cc. 1:1 CCl4-CHCl3 with ice bath cooling, the solvent removed, the residue taken up in Et2O, and the acidic fraction extracted from the solution gave XXVIII (R = H). XXVIII (R = H) (90 mg.) in 3 cc. AcOH treated with 200 mg. CrO3 in 3 drops concentrated H2SO4, kept 24 hrs., and diluted with H2O gave 20 mg. XVII, m. 208°. X (500 mg.) in 2 cc. AcOH treated with 2.0 g.

Na2Cr2O7 in 3 cc. AcOH followed by 4 drops concentrated H2SO4 and kept a few min. gave XXVIII (R = Me), m. 188-90° (C6H6-petr. ether, then sublimation in vacuo). XXVII (R = R' = Me) treated 1.5 hrs. with CrO2 in AcOH-H2SO4, diluted with H2O, and the precipitate filtered off gave crude XXVII (R = R' = Me), which contained a small amount petr. ether-insol. XXVIII (R = Me), m. 187-90° (C6H6).

IT 93536-38-0P, Spiro[2,5]octane-4-glyoxylic acid, 1-carboxy-4,8,8-trimethyl- 93865-03-3P, Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- 105912-69-4P, Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl-
RL: PREP (Preparation)
(preparation of)

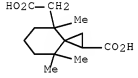
RN 93536-38-0 HCAPLUS

CN Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl-α-oxo- (CA INDEX NAME)



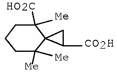
RN 93865-03-3 HCAPLUS

CN Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- (CA INDEX NAME)



RN 105912-69-4 HCAPLUS

CN Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl- (CA INDEX NAME)



L25 ANSWER 31 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1962:436487 HCAPLUS Full-text

DOCUMENT NUMBER: 57:36487

ORIGINAL REFERENCE NO.: 57:7317d-i,7318a-i,7319a-d
TITLE: The chemistry of the natural order cupressales. XL. The structure of thujopsene and hinokiic acid
AUTHOR(S): Norin, Torbjorn
CORPORATE SOURCE: Kungl. Tek. Hogskolan, Stockholm
SOURCE: Acta Chemica Scandinavica (1963), 15, 1676-94
CODEN: ACHSE7; ISSN: 0904-213X
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.

AB cf. CA 54, 24845e; 56, 6814a; 57, 3676a. Conclusive evidence is presented to establish the structures for thujopsene and hinokiic acid as I (R = Me and CO2H) (Ia and Ib, resp.), which, on catalytic hydrogenation, form the corresponding dihydro compds. (II) (R = Me and CO2H) (IIa and IIb, resp.) by conjugate addition of H. Proton magnetic resonance data had earlier confirmed the structures. Distillation of the neutral fraction of Japanese "hiba oil" gave Ia, b10 120°, [α]D -110° (C 2.0) (all rotations in CHCl3 unless otherwise stated), n25D 1.5031, d24 0.932. An acidic fraction (10 g.) from several Widdringtonia species was fractionally crystallized from Et2O and the more soluble material gave 0.5 g. Ib on recrystn. from Et2Opetr. ether (b. 40-60°) and then from MeOH, m. 169-70°, [α]D -86° (c 1.8). Recrystn. of the mother liquor residue from several solvents gave 4 g. of constant-melting material (m. 137-9°) which was chromatographed on silica gel with CHCl3-MeOH to give 3 g. Ib and 1 g. cuparenic acid, m. 158-60°, [α]D 63° (c 2.0). Oxidation of Ia with SeO2 gave I (R = CHO) (thujopsenal), m. 75-6°, [α]D -27° (c 1.9), which on Ag2O oxidation gave Ib. Ia (15 g.) in 200 ml. 6:1 EtOAc-MeOH was ozonized at -70° until a blue color appeared, the solution treated with N to remove excess O3 and the color, the mixture allowed to come to room temperature and treated, portionwise, with 30 g. Zn dust (activated with HOAc) to produce a vigorous reaction causing the mixture to boil. After 1 hr. the reaction was complete and 200 ml. Et2O was added, followed by 200 ml. 1% H2SO4, the mixture filtered, the Zn residue washed with Et2O, the organic phase separated, the H2O layer extracted with Et2O, the combined Et2O exts. washed with H2O, dried, evaporated, and the residue re-crystallized from EtOAc to give 11.5 g. crystalline 1-acetyl-4,4,8trimethylspiro[2.5]octane-8-acetic acid (III), m. 166-8°, [α]D -129° (c 2.0); semicarbazone m. 220° (decomposition); 2,4-dinitrophenylhydrazone m. 153-4°. The mother liquors yielded 1 g. addnl. III and 0.6 g. 1-hydroxyacetyl4,4,8-trimethylspiro[2.5]octane-8-acetic acid (IV), m. 193° (decomposition). III (250 mg.) in 2 ml. MeOH and 0.5 ml. 105% NaOH was added to 300 mg. KBH4 in 2 ml. MeOH and 4 ml. H2O, the mixture acidified, diluted with H2O till cloudy, warmed, the clear solution cooled to crystallize the product which was sublimed to give the lactone of 1-(1-hydroxyethyl)4,4,8-trimethylspiro[2.5]octane-8-acetic acid, m. 125-7°. III (5 g.) was dissolved in 50 ml. 10% NaOH and excess NaOBr solution (prepared from 25 g. NaOH, 400 ml. H2O and 9 ml. Br) at ice-bath temperature, the mixture kept 3 hrs. at room temperature and washed with Et2O, the solution decolorized with NaHSO3, acidified, extracted with Et2O, the Et2O extract washed with H2O and evaporated, and the residue recrystd. from EtOAc to give 4.5 g. 1-carboxy-4,4,8-trimethylspiro[2.5]octane-8-acetic acid (V), m. 215°, [α]D -57° (c 1.7). V was also obtained by hypoiodite oxidation of IV. V was converted into its anhydride by refluxing in Ac2O, m. 113° [CHCl3 petroleum ether (b. 40-60°)], [α]D 39° (c 2.4), and to its dimethyl ester (VI) with CH2N2, m. 71-3° (MeOH-H2O and sublimation), [α]D -59° (c 1.7). VI (2.82 g.), 30 ml. dry C6H6, and 0.54 g. NaOMe was refluxed 3 hrs. under N, cooled, poured into an ice-cooled mixture of 30 ml. Et2O and 60 ml. H2O, the layers separated, the H2O layer extracted with Et2O and acidified to give a low yield of V mono-Me ester (Va), m. 115-16° (MeOH-H2O). The combined organic extract was evaporated, the oily

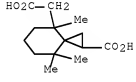
residue refluxed 2 hrs. in 20 ml. MeOH and 10 ml. 10% NaOH, the mixture cooled, diluted with H2O, acidified, extracted with EtO, the Et2O extract evaporated and the oily residue distilled in vacuo to give 1.72 g. crystalline VII (R = H2) (VIIa). Recrystn. from MeOH-H2O and sublimation in vacuo gave pure VIIa, m. 119-21° (sealed tube) (the crystals became isotropic at 49-50°), [α]D 65°; 2,4-dinitrophenylhydrazone m. 215-17°; semicarbazone m. 225-6° (decomposition). Ib was esterified with CH2N2 and the ester reduced with LiAlH4 to produce I (R = CH2OH) (VIII), m. 103-4° (petr. ether), [α]D 102°. VIII (0.3 g.) was ozonized to give 0.21 g. IV, m. 190-3° (decomposition) (Et2O-EtOAc). Ozonization of Ib followed by hypobromite oxidation gave VII (R = Br2) (IX), m. 99-100° (MeOH-H2O), [α]D 87deg;, V, and Va. IX (0.16 g.), 3 ml. HOAc, 1.0 g. Zn dust, and 0.5 g. NaOAc was refluxed 1 hr., filtered, the residue washed with Et2O, the filtrate washed with H2O and aqueous NaHCO3, dried, and evaporated to give 0.08 g. VIIa. VIIa was converted to IX, with Br in CCl3. IX failed to undergo dehydrobromination with LiBr in HCONMe2 or with collidine. VIIa (0.38 g.), 5 ml. HOAc, and 0.4 g. SeO2 was refluxed 1 hr., filtered to remove Se, the Se washed with Et2O, and the Et2O solution washed, dried and evaporated to give 0.4 g. orange oil which was chromatographed on Al2O3 to yield 0.15 g. VIIa and 0.17 g. VII (X = O) (X), m. (after sublimation in vacuo) 177° (sealed tube). X (0.15 g.) in 5 ml. MeOH and 5 ml. 10% KOH-MeOH was cooled (ice-bath), treated with 2 ml. 30% H2O2, stored overnight at 0°, refluxed 10 min., cooled, diluted with 20 ml. H2O to dissolve the white solid, acidified, extracted with Et2O, the Et2O extract dried and evaporated to give a solid which, after sublimation gave 0.14 g. crystalline anhydride (XI) of 1,8-dicarboxy-4,4,8-trimethylspiro[2.5]octane (XIa), m. 211-13° (sealed tube) (isotropic at 92-3°). XI was not hydrolyzed by rapid recrystn. from HOAc-H2O or recrystn. from MeOH-H2O. Slow crystallization of XI from HOAc-H2O gave crystalline XIa, m. 180° to an oil which resolidified to XI. Reduction of 0.5 g. VIIa in 6 ml. MeOH with 0.9 g. KBH4 in 15 ml. H2O and 6 ml. MeOH gave 0.425 g. XII (R = H) (XIIa), m. 133-5° (MeOH-H2O) (isotropic at 87°). VIIa (0.73 g.) with MeMgI gave 0.75 g. XII (R = Me) (XIII), m. 62-3° (MeOH-H2O). Se dehydrogenation of XIIa and XIII at 280-90° for 24 hrs. in CO2 atmospheric gave α-methyl- and 1,6-dimethylnaphthalene, resp., and tetrahydro compds. which, upon ozonization followed by H2O2 oxidation, produced α,α-dimethyladipic acid. Ia (4.04 g.) in 30 ml. MeOH and 3 ml. Et2O was hydrogenated over 10% Pd-C till 1 equivalent H had been absorbed, the mixture filtered, diluted with H2O, extracted with Et2O, and the Et2O extract dried and evaporated to give dihydrothujopsene (IIa), [α]D 24°, n25D 1.5100. Further hydrogenation proceededat a slower rate to give tetrahydrothujopsene, [α]D 27°, n25D 1.4922. Ib (0.469 g.) in 30 m. MeOH was hydrogenated over 10% Pd-C to give dihydrohinokiic acid (IIb), m. 158-60° (MeOH and sublimation), [α]D 75°. Hydrogenation of Ib with Pt-AcOH gave tetrahydrohinokic acid, m. 144-6° (MeOH), [α]D 60°. Ozonization of 4 g. IIa gave 3.1 g. 6-(2-oxobutyl)-1,2,2,6tetramethylcyclohexanecarboxylic acid (XIV), m. 160-1° (EtOAc), [α]D 71°, which on hypobromite oxidation gave 2.2 g. 6 - (2 - carboxyethyl) - 1,2,2,6 - tetramethylcyclohexanecarboxylic acid (XIVa), m. 185-7° (MeCN), [α]D -10°. IIb (0.5 g.) was ozonized to 0.31 g. aldehyde acid, m. 111- 13.5° (MeOH-H2O), which on Ag2O oxidation also gave XIVa. Dieckmann condensation of 1.42 g. of the di-Me ester of XIVa by refluxing 3 hrs. with 1 equivalent Nail in 20 ml. C6H6 gave 0.805 g. 3a,7,7,7a-tetramethylhexahydro-1-indanone (XV), m. 202° (sealed tube; crystals were isotropic at room a temperature), [α]D 82°. Attempts to prepare the 2,4-dinitrophenyl-hydrazone of XV failed. Quant. bromination expts. showed XV to contain only 2 α-H atoms and gave a dibromo ketone, m. 119-20°. Deuterium exchange also showed 2 α-Hatoms in XV. XV (100 mg.), 60 mg. KOD, 2.5 ml. D2O and 6 ml. dioxane was refluxed 30 min. under N, the mixture concentrated to 1/2 volume, cooled, extracted with petr. ether, the organic phase washed with D2O, dried, evaporated, and the crystalline residue (80 mg.) sublimed to give the α,α-dideuterio derivative of XV, m. 202°

(sealed tube). SeO2 oxidation of 0.3 g. XV gave 0.13 g. of the diketene, m. 125-6° (MeOH), which (0.1 g.) on oxidation with 2 ml. 30% H2O2 in 10 ml. 50% KOH-MeOH gave 0.7 g. 6-carboxymethyl-1,2,2,6-tetramethylcyclohex-anecarboxylic acid (XVI), m. 225-7° (decomposition) (MeOH-H2O), which on heating to the m.p. lost H2O and produced the anhydride of XVI, m. 216-18° (sealed tube; crystals be-came isotropic at 64°). Ia (0.741 g.) in 8 ml. MeOD and 2 ml. Et2O was deuteriated over 10% Pd-C (saturated with D) until 1 equivalent D had been taken up to give dideuterothujopsene (XVII), [α]D 22°, n25D 1.5013. Ozonization of XVII gave dideuterio derivative of XIV, m. 159-60°, which on OBr-oxidation gave the dideuterio derivative (XVIII) of XIVa, m. 185-7°. The di-Me ester of XVIII showed a decrease in intensity of the IR band at 1380 cm.-1 compared with that of the di-Me ester of XIVa. This proved that a new methyl group had been formed during hydrogenation of Ia. Ultraviolet and infrared data were given for the products.

IT 93865-03-3P, Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- 105912-69-4P, Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl-
RL: PREP (Preparation)
(preparation of)

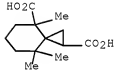
RN 93865-03-3 HCAPLUS

CN Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- (CA INDEX NAME)




RN 105912-69-4 HCAPLUS

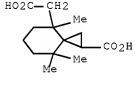
CN Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl- (CA INDEX NAME)



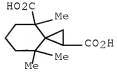

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L25 ANSWER 32 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1961:118650 HCAPLUS Full-text
DOCUMENT NUMBER: 55:118650
ORIGINAL REFERENCE NO.: 55:22362e-i,22363a-c
TITLE: Structure of thujopsene
AUTHOR(S): Nozoe, Tetsuo; Takeshita, Hitoshi; Ito, Sho; Ozeki, Takao; Seto, Shuichi
CORPORATE SOURCE: Tohoku Univ., Sendai
SOURCE: Chemical & Pharmaceutical Bulletin (1960), 8, 936-8

CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB Exptl. evidence was summarized in support of the structure B (Erdtman and Norin, CA 54, 24845e) versus A (Kobayashi, et al., CA 54, 2403c) for thujopsene (I). Ozonolysis of I gave the oxo acid (II), m. 164°; 2,4-dinitrophenylhydrazone (III) m. 197°. II treated with acid at 0° gave the oxo-γ-lactone (IV), m. 56°; 2,4-dinitrophenylhydrazone (V) m. 164°. Hypobromite oxidation of II gave the dicarboxylic acid (VI), m. 212°, which had 2 isomeric monomethyl esters, m. 59-60° and 114-15°, formed, resp., by mild esterification of VI and partial hydrolysis of the dimethyl ester of VI, m. 73°. Permanganate oxidation of I gave both II and the lactol-ketal (VII), m. 123°. CH2N2 with VII gave the Me ester (VIII) of a diketo acid, m. 89°, whereas alkaline treatment of VII gave the hydroxyoxocarboxylic acid (IX), m. 212°, which was dehydrated and decarboxylated to the unsatd. ketone (X), m. 75°; 2,4-dinitrophenylhydrazone (XI) m. 173-4° and 177-8°, 2 compds. with the same ultraviolet spectrum. Catalytic hydrogenation of X gave the corresponding saturated ketone (XII), m. 105°; [α]306 4890°; 2,4-dinitrophenylhydrazone (XIII) m. 187°. Ozonolysis of X gave the nordicarboxylic acid (XIV), m. 212°, also formed from VI through its cyclic ketone (XV), m. 120°, [α]302 7030°. Ultraviolet absorption data were, listed for II-V, X-XIII, and XV, and infrared data for II, IV, VII, VIII, X, XII, and XV. All evidence led to acceptance of the structure B for I.
IT 93865-03-3P, Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl-, methyl esters 105912-69-4P, Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl-
RL: PREP (Preparation)
(preparation of)
RN 93865-03-3 HCAPLUS
CN Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- (CA INDEX NAME)

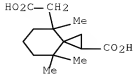


RN 105912-69-4 HCAPLUS
CN Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl- (CA INDEX NAME)

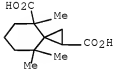


OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)

L25 ANSWER 33 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1960:129301 HCAPLUS Full-text
DOCUMENT NUMBER: 54:129301
ORIGINAL REFERENCE NO.: 54:24845d-i,24846a-c
TITLE: Structure of thujopsen and hinokiic acid
AUTHOR(S): Erdtman, H.; Norin, T.
CORPORATE SOURCE: Kgl. Tek. Hogskolan, Stockholm
SOURCE: Chemistry & Industry (London, United Kingdom) (1960) 622-3
CODEN: CHINAG; ISSN: 0009-3068
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 22 Apr 2001
GI For diagram(s), see printed CA Issue.
AB Thujopsen (I, R, = H) (II) ozonized gave III, m. 168°, which was further oxidized to IV, m. 215°, which easily gave V, m. 114°, by a Dieckmann condensation. V with SeO2 followed by H2O2 gave VI, which on heating gave a stable 6-membered ring anhydride, m. 211°, possessing a rigid spirocyclic structure. IV with Ac2O gave a 7-membered ring anhydride, m. 113°. V with NaBH4 gave the alc., m. 133°, which dehydrogenated with Se gave α-methylnaphthalene and a tetrahydronaphthalene derivative which with O3, then H2O2, gave α,α-dimethyladipic acid (VII). V with MeMgI gave VIII, m. 63°, which dehydrogenated with Se gave 1,6-dimethylnaphthalene and a tetrahydronaphthalene derivative which was oxidized to VII as before. V contained a CO group conjugated with a cyclopropane ring, but the infrared spectrum of the anhydride of IV (but not of VI) indicated a -CH2- group adjacent to CO. Hydrogenation of II (MeOH-Et2O, Pd-C) gave IX (R = Me) (X). Further hydrogenation gave tetrahydrothujopsen. X with O3 gave an oxocarboxylic acid, C15H26O3, m. 160-1°, further oxidized to a dicarboxylic acid, C14H24O4 (XI), m. 188°, which by Dieckmann condensation readily gave XII, m. 202°. None of these 3 compds. showed ultraviolet absorption, indicating the presence of a cyclopropane ring conjugated with CO. Similarly, hinokiic acid (I, R = CO2H) (XIII) gave XI, m. 188°, via IX (R = CO2H) (XIV), m. 160°. II and XIII exhibit infrared absorption at 1380 cm.-1, which band strongly increased in the dihydro derivs.; this conformed with the appearance of a new Me group after hydrogenation. Proton magnetic resonance (PMR) studies on II, XIII and their derivs. confirmed the structure II; 3 protons were found at the cyclopropane ring in the anhydride of VI. The PMR spectra of X and XIV showed a prominent line corresponding to an addnl. angular Me group; olefinic H atoms gave rise to 1 sharp line indicating the presence of .tpl.bond.CCH:C:. V exhibited a strong pos. Cotton effect. Application of the octant rule to V thus suggested that the cyclopropane ring stands out from the plane of the paper.
IT 93865-03-3P, Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- 105912-69-4P, Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl-
RL: PREP (Preparation)
(preparation of)
RN 93865-03-3 HCAPLUS
CN Spiro[2.5]octane-4-acetic acid, 1-carboxy-4,8,8-trimethyl- (CA INDEX NAME)



RN 105912-69-4 HCAPLUS
CN Spiro[2.5]octane-1,4-dicarboxylic acid, 4,8,8-trimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

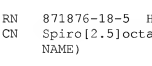
L25 ANSWER 34 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1932:33661 HCAPLUS Full-text
DOCUMENT NUMBER: 26:33661
ORIGINAL REFERENCE NO.: 26:3489b-i
TITLE: Chemistry of alkylcyclopentanones. II. Effect of the methylcyclopentane ring on the carbon tetrahedral angle
AUTHOR(S): Desai, Ranchhodji Dajibhai
SOURCE: Journal of the Chemical Society (1932) 1065-79
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB cf. C. A. 25, 4234. The results obtained, in the decomposition of the mono- and di-Br esters of 3-methylcyclopentane-1,1-diacetic acid show that the methylcyclopentane ring bears the closest similarity to the cyclopentane ring and differs fundamentally from the cyclohexane nucleus. If the effect of this ring were due to polar factors, it should be similar to the gem-EtPr group; the effect is, however, more in harmony with that of the gem-Me2 group and is due to valency deflection. Et H 3-methylcyclopentane-1,1-diacetate yields the anhydride on distillation The α-Br derivative (I), b7 163°, results in 80% yield; 3 distns. give the lactonic ester, b20 188°; the mono-Br acid ester is a dark yellow viscous oil. Hydrolysis of I with KOH at 150° gives trans-3-methylcyclo pentanespirocyclopropane-2',3'-dicarboxylic acid A, m. 230° (dianilide, m. 295°), and the acid B, m. 215° (dianilide, m. 275°); the Et2O solution from the above acids gives the cis-anhydride A, m. 75°, from which was prepared the cis-acid A, m. 175°; anilic acid, m. 190°. Heating I with Na2CO3 for 72 hrs. gives the lactonic acid A (of-α -hydroxy-3-methylcyclopentane-1,1-diacetic acid), m. 87°; aniline salt, m. 95°. The acid ester, similarly treated for 12 hrs., gives the lactonic acid B, m. 75°. The α,α'-di-Br ester (II) is a reddish yellow viscous liquid; the Et H ester m. 128° Distillation of II gives the lactone of Et H α-bromo-α'-hydroxy-3-

methyl- cyclopentane-1,1-diacetate, b15 195-6°. The α,α'-dibromo-3-methylcyclopentane-1,1-diacetic acids m. 195° (decomposition) and 163°. Hydrolysis of II with KOH gives α-keto-3-methylcyclopentane-1,1-diacetic acid, m. 121° (quinoxaline derivative, m. 226-7°; 2,4-dinitro-phenylhydrazone, S-yellow, m. 185° (decomposition); Me ester, b19 169°, whose phenylhydrazone m. 163°), and a small quantity of the trans-lactone of the di-HO acid, m. 146°. Oxidation of keto acid gives 1-carboxy-3-methylcyclopentane-1-acetic acid, m. 120°, which was also prepared from 3-methylcyclopentanone cyanohydrin, b25 128-30°. Methylcyclopentanone, BrCH2CO2Et and Zn give 25-30% of Et 3-methylcyclopentan-1-ol-1-acetate, b20 121°; free acid (III), m. 56; 20-5% of the ketone underwent self-condensation, giving 4-methyl-2-(3'-methylcyclopentylidene)cyclopentanone, b2, 132-3°, d420 0.9552, nD20 1.4964; semicarbazone, m. 142-3°. Heating III with AC2O 4 hrs. gives 3-methylcyclopentylideneacetic acid, m. 112°. Hydrolysis of II with MeOH-KOH gives trans-3-methylcyclopentanespiro-2'-methoxycyclopropane- 2',3'-dicarboxylic acid A, m. 190°, and B, m. 178°; the lactone of the α-hydroxy-α'-methoxy acid m. 150°; the cis-methoxyspiro acid A m. 175°, and its anhydride m. 87°; the B acid m. 162° and its anhydride m. 60°. The α-hydroxy-α'-methoxy acid m. 145°. Heating the Et H ester of the di-Br acid with Na2CO3, gives the trans-lactone, m. 146° (Ac derivative, m. 151°), and the cis-isomer, m. 125°, of α,α'-dihydroxy-3-methylcyclopentane-1,1- diacetic acid. Me 3-methylcyclopentane-1,1-diacetate, b15 137°, and (CO2Me)2 with Na in Et2O give Me 3-methylcyclopentanespiro-3',4'- diketocyclopentane- 2',5'-dicarboxylate, m. 125°; FeCl3 gives a red color; semi-carbazone, m. 182°; heating with 20% H2SO4 gives 3-methylcyclopentanespirocyclo-pentane-3',4'-dione, m. 108° (disemicarbazone, m. 245° (decomposition)). The acid chloride of Et 1-carboxy-3-methylcyclopentane-1-acetate and MeZnI give the Et ester, b11 135°, d416 1.008, nD16 1.45723 (semicarbazone, m. 105°), of 1-acetyl-3-methylcyclopentane-1-acetic acid, m. 83° (semicarbazone, m. 200°). The ester with EtONa gives 20% of 3-methylcyclopentanespirocyclopentane-2',4'-dione, m. 101° (Br derivative, m. 185°).

IT 871876-17-4, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-6-methyl- 871876-18-5, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-5-methyl- 871876-19-6, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-4-methyl-
(isomers and derivs.)

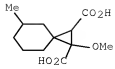
RN 871876-17-4 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-6-methyl- (CA INDEX NAME)

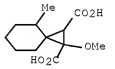



RN 871876-18-5 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-5-methyl- (CA INDEX NAME)




RN 871876-19-6 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-4-methyl- (CA INDEX NAME)




L25 ANSWER 35 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1932:33660 HCAPLUS Full-text
DOCUMENT NUMBER: 26:33660
ORIGINAL REFERENCE NO.: 26:3488a-i,3489a-b
TITLE: Formation and stability of spiro compounds. XIV. Effect of the methylcyclohexane ring on the carbon tetrahedral angle
AUTHOR(S): Desai, Ranchhodji Dajibhai
SOURCE: Journal of the Chemical Society (1932) 1047-65
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB The recent work of Rao (C. A. 24, 4022) and Kandiah (C. A. 25, 3334) has shown that when cyclohexane is interlocked in the o-position with a 6- or 5-membered ring, the resulting dicyclic nuclei behave like strainless rings. The present study of the decomposition products of the mono-Br and di-Br esters of 3- and 4-methylcyclohexane-1,1-diacetic acids shows that the methylcyclohexane ring simulates the behavior of strainless rings such as cyclopentane and especially trans-decalin and hexahydrohydrindene; the question, "How is this strain relieved?" is discussed. The ω-imide of 4-methylcyclohexane-1,1-dicyanoacetic acid on hydrolysis with hot dilute $H_2SO_4$ gives 4-methylcyclohexane-1, 1-diacetic acid (I), but with cold concentrated $H_2SO_4$ there results the ω-imide of 4-methylcyclohexane-1,1-dicarbamylacetic acid, m. 260° (decomposition). The Et ester of I b24 178°. The anhydride of I and $PhNH_2$ give 2 anilic acids, separated by crystallization from EtOH, m. 184° and 148°; only 1 anil, m. 140°, was formed. The anhydride and EtONa-EtOH give the Et H ester of I, viscous oil, yielding the anhydride on distillation This ester with $PCl_6$ and Br at 50-60° gives 75% of Et-α-bromo-4-methylcyclohexane-1,1-diacetate (II), which loses EtBr on distillation, giving the lactonic ester, b20 205°. The mono-Br acid ester is a dark yellow, viscid oil. Hydrolysis of II with 64% KOH at 150° gives a mixture of the trans-4-methylcyclohexanespirocyclopropane-2',3'-dicarboxylic acid, m. 212°, and the cis-acid, m. 165°, separated by heating with AcCl for 12 hrs.; the anhydride

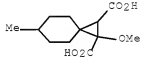
from the cis-acid m. 72°. A small quantity of a lactone acid, m. 145°, was isolated. The trans-spiro acids of this and the m-series are stable to 5% HCl at 240° and to 10% HCl at 200° but are decomposed by the latter at 240° and by 20% HCl at 200°. I, PCl5 and Br, heated at 50-60° and poured into EtOH, give 85% of Et α, α'-dibromo-4-methylcyclohexane-1,1-diacetate (III), which yields the bromolactonic ester, b21 235°, on distillation The acid product of the dibromination was a semi-solid mixture of di-Br and mono-Br acid esters, separated by extraction with C6H6-petroleum. Warming the di-Br acid chloride with HCO2H for 4 hrs. gives the lactone α-bromo-α'-hydroxy-4-methylcyclohexane-1,1-diacetic acid, m. 210°, and also the, α,α'-di-Br derivative of I, m. 185° (decomposition). Hydrolysis of III with 64% KOH at 150° gives a small quantity of 4-methylcyclohexenylacetic acid, m. 42-3°; α-keto-4-methylcyclohexane-1,1-diacetic acid A, m. 147° (insol. in C6H6); quinoxaline derivative, m. 226°; 2,4-dinitrophenylhydrazone, S-yellow, m. 220°; Me ester, b25 192° (phenylhydrazone, m. 163°); the C6H6, extract gave the keto acid B, m. 128-9°; quinoxaline derivative, m. 245°; 2,4-dinitrophenylhydrazone, S-yellow, m. 205° (decomposition phenylhydrazone, m. 204° (decomposition); Me ester, b20 187° phenylhydrazone, m. 227° (decomposition). Oxidation of A with alkaline H2O2 gives 1-carboxy-4-methylcyclohexane-1-acetic acid A, m. 136° the B isomer m. 173° (decomposition) and yields an anhydride, m. 104°, and an anilic acid, m. 184°. Hydrolysis of III with MeOH-KOH by heating 20 min., refluxing the acids with AcCl and extracting the Et2O solution with 5% NaHCO3 gives the anhydride A, m. 148°, of IV and from the petroleum extract, anhydride B, m. 90°. The anhydride A gives the anilic acids A and B, m. 183° and 160°, and give the same anil, m. 134°. Anilic acids A' and B', m.193° (decomposition) and 157°, precipitated at once when the anhydride B and PhNH2 were mixed in C6H6; the anil m. 96°. Anhydride A gives cis-4-methylcyclohexanespiro-2'-methoxycyclopropane- 2',3'-dicarboxylic acid A (IV), m. 182° (decomposition); the cis-acid B m. 162° (decomposition). The NaHCO3 extract gives the trans-acid A, m. 190°, which gives the cis-anhydride A on distillation IV and HBr, refluxed 6 hrs., give 1-carboxy-4-methylcyclohexane-1-acetic acid, m. 173°, and α-keto-4-methylcyclohexane-1,1-diacetic acid B, m. 129°; the cis-acid B gave the keto-acid A, m. 147°. The ω-imide of 3-methylcyclohexane-1,1-dicarbamylacetic acid m. 272° (decomposition). Et 3-methylcyclohexane-1,1-diacetate (V) b22 174°; the anilic acids A and B m. 172° and 141°; the anil m. 137°. Et a-bromo-3-methylcyclohexane-1,1-diacetate (VI) results in 75% yields and on distillation gives the lactonic ester, b16 196°; the mono-Br acid ester is a dark yellow viscous liquid. Hydrolysis of VI with 64% KOH at 150° gives trans-3-methylcyclohexanespirocyclopropane-2',3'- dicarboxylic acid A, m. 270° (dianilide, m. 280°); the more soluble transacid B m. 245° (dianilide, m. 260°); the cis-acid A m. 205°. The α,α'-di-Br derivative of V results in 85% yield and on distillation gives the Br lactonic ester, pale yellow, b21 234°, m. 130°; the Et H ester m. 162°. The gum obtained by decomposing the di-Br acid chloride with HCO2H gives a mixture of the Br lactonic acid A, m. 225°, and B, m. 201°. Hydrolysis of the di-Br ester with KOH at 150° gives 3-methylcyclohexenylacetic acid, b20 152-3 ° α-keto-3-methylcyclohexane-1,1-diacetic acid A m. 139-40° (quinoxaline derivative, m. 217°; 2,4-dinitrophenylhydrazone, yellow, m. 198°); the more soluble (in C6H6) keto acid B m. 126-7° (quinoxaline derivative, m. 239°; 2,4-dinitrophenylhydrazone, S-yellow, m. 194° (decomposition); the Me ester, b23 185°, gives a phenylhydrazone, m. 220° (decomposition)). Oxidation of the acid B with H2O2 gives 1-carboxy-3-methylcyclohexane-1-acetic acid, m. 163° (decomposition); the anhydride b22 166°, m. 41° ; anilic acid, m. 170° (decomposition); anil, m. 139°. Hydrolysis with MeOH-KOH gives cis-3-methylcyclohexanespiro-2-°-methoxycyclopropane-2',3'- dicarboxylic anhydride A, m. 140-1°; the anhydride B m. 116°, anhydride C m. 101° and anhydride D m. 85°; anilic acid A, m. 195° (decomposition), and B, m. 135°, and anil, m. 112°, were prepared from anhydride A; the cis-MeO acid A m. 194° (decomposition). The cis-anhydride B

gives an anilic acid, m. 215° (decomposition); the cis-MeO acid B m. 195° (decomposition). Anhydride C gives an anilic acid, m. 212°; the cis-MeO acid C m. 197° (decomposition). Anhydride D gives an anilic acid, m. 192° (decomposition), and an anil, m. 118°; the cis-MeO acid D m. 196° (decomposition). trans-3-Methylcyclohexanespiro-2'-methoxycyclopropane-2',3'-dicarboxylic acid A m. 201°; distillation gives the cis-anhydride A.

IT 871876-17-4, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-6-methyl- 871876-18-5, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-5-methyl- 871876-19-6, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-methoxy-4-methyl- (isomers and derivs.)

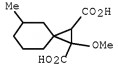
RN 871876-17-4 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-6-methyl- (CA INDEX NAME)



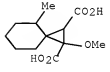

RN 871876-18-5 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-5-methyl- (CA INDEX NAME)




RN 871876-19-6 HCAPLUS

CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-methoxy-4-methyl- (CA INDEX NAME)




L25 ANSWER 36 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN

ACCESSION NUMBER: 1924:2605 HCAPLUS Full-text

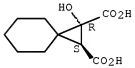
DOCUMENT NUMBER: 18:2605

ORIGINAL REFERENCE NO.: 18:379b-i,380a-b

TITLE: Ring-chain tautomerism. VIII. The effect of the

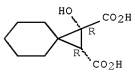
cyclohexane nucleus on the carbon tetrahedral angle
AUTHOR(S): Lanfear, E. W.; Thorpe, J. F.
SOURCE: Journal of the Chemical Society, Transactions ( 1923), 123, 2865-70
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
AB Hydrolysis of Et α,α'-dibromocyclohexane-1,1-diacetate (C. A. 9, 3059) gave a mixture of the trans- and cis-cyclohexanespiro-1-hydroxycyclopropane-1,2-dicarboxylic acids (I and II), the former of which m. 217° and was identical with that previously obtained from the bromolactone, while the latter m. 163°. Ag2 salts. Warming II with AcCl gave the anhydride, m. 102°, reconverted into II by dilute alkali. Concentrated HBr, with either I or II gave α-ketocyclohexane-1,1-diacetic acid, m. 130°. In the case of I, the bromolactonic acid, m. 161°, was also formed. The keto acid is completely converted into the K salt of I by boiling 0.5 hr. with concentrated aqueous KOH. These facts complete the chain of proofs advanced for the hypothesis regarding the C tetrahedral angle.
IT 1194718-54-1P 1194759-71-1P
RL: SPN (Synthetic preparation); PRP (Properties); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(Ring-chain tautomerism. VIII. The effect of the cyclohexane nucleus on the carbon tetrahedral angle)
RN 1194718-54-1 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-hydroxy-, (1R,2S)-rel- (CA INDEX NAME)

Relative stereochemistry.




RN 1194759-71-1 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-hydroxy-, (1R,2R)-rel- (CA INDEX NAME)

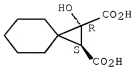
Relative stereochemistry.




IT 904818-53-7P, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-hydroxy-, cis- 904833-38-1P, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-hydroxy-, trans-
RL: PREP (Preparation)
(preparation of)

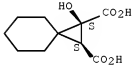
RN 904818-53-7 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-hydroxy-, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.




RN 904833-38-1 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1-hydroxy-, (1S,2S)- (CA INDEX NAME)

Absolute stereochemistry.



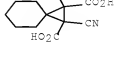

L25 ANSWER 37 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1921:20457 HCAPLUS Full-text
DOCUMENT NUMBER: 15:20457
ORIGINAL REFERENCE NO.: 15:3825b-i,3826a
TITLE: Formation and stability of spiro compounds. VI. New derivatives of cyclopropane and cyclohexanespirocyclopropane
AUTHOR(S): Birch, Stanley Francis; Henry, William; Kon, George Armand Robert
CORPORATE SOURCE: Imp. Inst. Sci. Tech., South Kensington
SOURCE: Journal of the Chemical Society, Transactions ( 1921), 119, 1315-28
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
GI For diagram(s), see printed CA Issue.
AB In searching for possible new sources of cyclopropane derivs. it has been found that the bridged piperidine compds. of Guareschi (C. A. 6, 865) on regulated hydrolysis with alkali furnish such a source. 2,3-Dicyano-I,I-dimethlcyclopropane-2-corboxamide (H), is obtained by boiling with 10% KOH (1 mol.) for 5 min. and then cooling, long flattened needles from dilute alc. or C6H6, m. 163.5°. The acid, C8H8O2N2 (U), is obtained when 5 g. H in 100 cc. cold concentrated H2SO4 are treated with saturated NaNO2 in H2O until the mixture is nearly solid. The product is poured into H2O, extracted with Et2O and the acid removed with Na2CO3. It forms large transparent rhombic laminas, m. 168-9°, from H2O. The acid may also be obtained by boiling the imide with 5% KOH for 1 hr. The mother-liquors from j contained terebic acid and a

compound, HOCMe2CH(CN)CH(CN)CO2H (?), forming fine, long needles from H2O and m.234-5°. J, heated with a little water in a sealed tube for 1 hr. at 180-200°, gave, 1,1-dimethyZcyclopropane-2,3-dinitrile, C7H8N2, b12 158°, long, flattened needles, m. 50°. Boiled with alc. KOH, a mixture of cis- and trans-caronic acids was obtained (Beesley, Ingold, and Thorpe, CA. 9,3059). When 3.8g.H are heated with 6g. KOH in 45 cc. H2O for 3-4 hrs., β-hydroxy-β-methylbutane- αδ,δ-tricarboxylic lactone (K), C8H10O6, is formed, large prisms from a small amount H2O (in which it is very soluble), m. 157°. Silver salt, very soluble in H2O. Warmed with 25% H2SO4, the lactone loses 1 CO2 and gives terebic acid (J. Chemical Society 75, 48). α,β-Dicyano-α-hydroxy-α-methylbutane-α,β- dicarboxylic acid (L), Me2C(OH)C(CN)(CO2H)CH(CN)CO2H, prepared by heating the imide with 3 mols. aqueous KOH for 0.5 hr. and then acidifying, thick, transparent rhom- bic plates from H2O, m. 195-6° (decomposition). With 50% H2SO4 the acid is decomposed into (HO2CCH2)2 and AcMe. The action of concentrated KOH on the imide gave K. Cyclohexanespiro-2,3-dicyanocydopropane-2- carboxamide, C11H12ON3, from the spiro-imide as above, fine, glistening plates or felted needles from dilute alc or C6H6 141°. The acid, C11H12O2N2, prepared by the action of NaNO2 on the amide or by direct hydrolysis of the spiro-imide with 2 mols. KOH, forms prisms, m. 159°, best from 50% HCl. Cydohexanesirocyclopropane-2,3-dinitrile, C10H12N2, lustrous plates, m. 86°, which, on hydrolysis, gave cyclohexanespirocyclopropane-2,3-dicarboxylic acid (B., I. and T.) 1-Hydroxycyclohexylethane-α,β,β-tricarboxylic α-lactone, C11H14O6 (M), by heating the amide with 15% KOH for 4 hrs., spherical aggregates of buff-colored crystals, m. (not sharply) 183-4° , which is probably the trans-isomer since it is not affected by boiling AcCl. Silver salt. On heating above the m. p., or on boiling with 20% H2SO4, the α-lactone of the α,β-dicarboxylic acid (N) is formed, plates from H2O, m. 184-5° Silver salts, both of the lactonic acid and the dibasic HO acid, were prepared N is stable to KMnO4. Anilide, C15H19ON, iridescent plates, m. 113°. In its formation I H2O and 1 CO2 appear to be eliminated. Cyclohexanespiro-2,3-dicyanocyclopropane-2,3-dicarboxylic acid, C12H12O4N2, by boiling a solution of the spiro-imide in 3 mols. 10% KOH for 30-40 min., small plates from dilute alc., m. and decompose 207°. Anhydride, by heating above the m. p.of the acid for 20 min., colored crystals, m. 99°. When an excess of KOH is used in the hydrolysis, cyclohexanespiro-2-cyanocyclopropane-2,3,3-tricarboxylic acid, C12H13O6N, results, stellate clusters of prisms, m. 169° (decomposition). The potassium hydrogen salt forms needles from alc., m. 237° (decomposition).

IT 861368-12-9P, 3,6-Spirooctane-1,1,2-tricarboxylic acid, 2-cyano-
861515-57-3P, 3,6-Spirooctane-1-carboxamide, 1,2-dicyano-
861564-55-8P, 3,6-Spirooctane-1,2-dicarboxylic acid, 1,2-dicyano-
861564-58-1P, 3,6-Spirooctane-1-carboxylic acid, 1,2-dicyano-
RL: PREP (Preparation)
(preparation of)

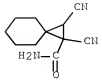
RN 861368-12-9 HCAPLUS

CN Spiro[2.5]octane-1,1,2-tricarboxylic acid, 2-cyano- (CA INDEX NAME)

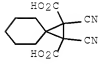



RN 861515-57-3 HCAPLUS

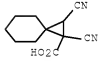
CN Spiro[2.5]octane-1-carboxamide, 1,2-dicyano- (CA INDEX NAME)



RN 861564-55-8 HCAPLUS
CN Spiro[2.5]octane-1,2-dicarboxylic acid, 1,2-dicyano- (CA INDEX NAME)



RN 861564-58-1 HCAPLUS
CN Spiro[2.5]octane-1-carboxylic acid, 1,2-dicyano- (CA INDEX NAME)



L25 ANSWER 38 OF 38 HCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1915:18519 HCAPLUS Full-text
DOCUMENT NUMBER: 9:18519
ORIGINAL REFERENCE NO.: 9:3059h-i,3060a-i,3061a-h
TITLE: Formation and stability of spiro-compounds. I. Spiro-compounds from cyclohexano
AUTHOR(S): Beesley, Richard M.; Ingold, Christopher K.; Thorpe, Jocelyn F.
SOURCE: Journal of the Chemical Society, Transactions ( 1915), 107, 1080-1106
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
ED Entered STN: 16 Dec 2001
GI For diagram(s), see printed CA Issue.
AB A series of investigations has been undertaken with the object of ascertaining "the effect produced by the alteration of the tetrahedral angle consequent on ring formation, on the formation and stability of a 2nd ring joined to the existing ring by a quaternary C atom common to both." The hypothesis was advanced that the angle formed by the 2 side chains attached to any 1 C atom of the cyclohexane ring will be altered in proportion to any change in angle between those valencies which participate in ring formation; i. e., the groups attached to 2 side chains emanating from the same C atom of a cyclohexane

derivative, type (I), will be closer together than in a corresponding compound having the open chain structure, type (II). Expts. show that this hypothesis is probably correct. For example a trans-spiro-acid, derived from a compound of type (I) is more stable than trans-caronic acid, derived from a compound of type (II). The above hypothesis and another untenable one are presented and discussed in some detail and diagrammatically represented by showing the effect of "strain" on the angles between the valencies (represented by the apices of an inscribed tetrahedron) of a (spherical) C atom. The bromination of CH2(CH2)4C(CH2CO2H)2 by means of PBr5 and Br led to the formation of a mixture containing an acid product, probably C5H10>C(CHBrCO2H)(CH2CO2Et) (A), and a neutral product (B). The latter was shown to be a mixture of cis-diethyl α,α'-dibromocyclohexane-1,1-diacetate (C) (not obtained in the pure state) and the trans-lactone (D), C5H10>C.CH(CO2Et).O.CO.CHBr, prisms from petroleum or alc., m. 96°, b20 225-30°. (D) was separated from the mixture (B) by the addition of an equal volume of petroleum (b. 60-70°) and was also synthesized by boiling (C) with C5H5N [whereby only the trans-form of (C) was converted into (D)] or by distilling (C), whereby both the cis- and trans-forms were converted. The isomeric cis-lactone (D'), microneedles, m. 69-70°, was formed in 25% yield upon distilling (C) from which (D) had been previously removed by means of C5H5N. α-Hydroxycyclohexane-1,1-diacetic acid lactone (E), C5H10>C.CH(CO2H).O.CO.CH2, b13 240-1°, crystallizing after long standing and seeding, microneedles, m. 91-2° (silver salt, amorphous), was formed from (A) by the action of boiling Na2CO3. The free acid (F) corresponding to (E) could not be isolated and was found to be stable only in the form of its salts. The amorphous silver salt and crystalline sodium salt of (F) were prepared The dianilide of (F), C5H10>C(CH2CONHPh)CH(OH)CONHPh, needles, m. 97°. The aniline salt of (E), silky needles, m. 104°. When (A) was added to boiling concentrated KOH and the reaction mixture cooled and acidified, trans-cyclohexane-spiro-cyclopropane-1,2-dicarboxylic acid (G), C5H10>C.CH(CO2H).CHCO2H, flattened needles, m. 237°, was formed. Its silver salt separated in the form of a crystalline powder: its dianilide, needles, m. 292°. The filtrate from (G) after extraction with Et2O and fractionation under reduced pressure yielded the cis-isomer (H) of (G), needles, m. 198°, more readily formed by distilling (G) which is first converted into the anhydride (J), C5H10>C.CH.CO.O.CO.CH, needles, m. 102°, which on treatment with alkali and subsequent acidification yields (H). (J) was also readily prepared by the interaction of (H) and AcCl, whereas (G) is not acted upon by this reagent. The anilic acid, C5H10>C.CH(CO2H).CHCONHPh, derived from (J), small needles,m. 207° (decomposition); the corresponding anil, m. 119°. When heated in a sealed tube with 50% concentrated HCl at 180° for 5 hrs., (H) is partially reconverted into (G). On attempting to replace the Br in (D) by an OH group, by means of moist Ag2O, ethyl α-hydroxycyclohexane-1,1-diacetate lactone, C5H10> C.CH2CO.O.CHCO2Et, b21 210°, was obtained and yielded (E) on hydrolysis. The following hydrolysis products were formed when (D) was treated with boiling 15% aqueous NaOH:C5H10>C:CHCO2H (K), m. 92° (identical with Wallach's acid as shown by the formation of the dibromide, m. 135-6°; reference not given), and the trans-lactonic acid of α,α'-dihydroxycyclohexane-1,1-diacetic acid (L), C5H10>C.CH(OH).CO.O.CHCO2H.H2O, prisms, 100°, anhydrous, m. 145°. (D') when subjected to a similar hydrolysis gave rise to a mixture of (K), the cis-isomer (M) of (L), prisms, m. 168°, and cyclohexane-spiro-cyclopropanol-2,3-dicarboxylic acid (N), C5H10>C.C(OH)(CO2H).CHCO2H, pearly plates, m. 217°. Boiling alc. KOH, reacting with (D), yielded (K), (L) and (N). The action of 64% aqueous KOH on (D) gave rise to a mixture of (L), (N) and Δ1-cyclohexeneacetic acid, (O), CH2(CH2)3CH:C.CH2CO2H, m. 38° (identical with Wallach's compound; also quant. formed by boiling (K) with 64% KOH, thus indicating that it was a byproduct in the above reaction). The Et ester of (O), b25 118-2° (cf. Auwers and Ellinger, C. A. 6, 1147). A similar reaction between 64% KOH and (D') gave rise to (O), (M) and (N). (K) and (N) were separated by treatment with dry

Et2O in which (N) is insol. (L) was ordinarily separated from hydrolysis mixts. by esterifying and fractionating the ethyl ester, b25 206-10°. The following derivs. of (L) are described: disodium salt, crystalline; disilver salt, powder; aniline salt, microcrystals, m. 133-4°; dianilide, C5H10>C[CH(OH)CONHPh]2, short needles, m. 169°. (L) does not react with AcCl, is not reduced by AgOH, and when heated with H2O in a sealed tube or when distilled, passes into (M). The isolation of (M) was effected by esterifying hydrolysis mixts. and collecting the fraction of highest b. p., which was subsequently hydrolyzed with HCl. (M) was readily acetylated. The following derivs. of (M) were prepared: disilver salt; dianilide, needles, m. 169° (not identical with the dianilide derived from (L)); acetate, C5H10>CH(OAc).CO.O.CHCO2H, m. 156° (silver salt of the acetate, crystalline powder). The spiro-acid (N), which like (L) could not be acetylated, which is not converted into the lactone on heating and is otherwise stable, gave rise to the following compds.: silver salt, crystalline powder; anilide, needles, m. 202°. Concentrated H2SO4 acting upon (L) at 95-100°, gave rise to small amts. of cyclohexane-spiro-cyclopentanone, oil (forming a semicarbazone, needles, m. 175°), and an unidentified compound, m. 105°. When heated with an equal amount of H2O in a sealed tube at 240° for 0.5 hr., (L) yielded the lactonic acid of α-hydroxy-α'-cyclohexan-1- olsuccinic acid, C5H10>C.O.CO.CH(OH).CHCO2H, cubical prisms, m. 131°, whose disodium salt, disilver salt and aniline salt, m. 123°, were prepared

IT 67911-20-0, 3,6-Spirooctane-1,2-dicarboxylic acid, trans-
68194-50-3, 3,6-Spirooctane-1,2-dicarboxylic acid, cis-
860756-70-3, 3,6-Spirooctane-1,2-dicarboxylic acid, 1-hydroxy-
(and derivs.)

RN 67911-20-0 HCAPLUS

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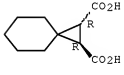
Relative stereochemistry.

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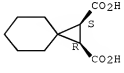
Relative stereochemistry.

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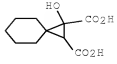

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RL: PREP (Preparation)
(preparation of)
RN 859961-01-6 HCAPLUS
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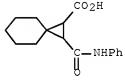

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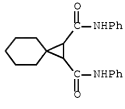

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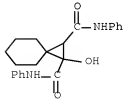

OS.CITING REF COUNT: 173 THERE ARE 173 CAPLUS RECORDS THAT CITE THIS RECORD (173 CITINGS)

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